Mixed valence as an almost broken symmetry

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By using a generalized version of the infinite-U Anderson model, strong-coupling properties of mixed-valence systems are modeled by means of an expansion about a broken-symmetry mean-field theory. A renormalized Fermi liquid, with heavy-fermion bands in the lattice is an intrinsic feature of this mean-field theory. Strong-coupling divergence of the Kondo coupling constant arises as a direct consequence of the zero-mode fluctuations about the broken-symmetry state. In the large-degeneracy limit these fluctuations vanish and the broken-symmetry state is an exact solution, explicitly confirmed for the single-impurity case by a new Bethe-ansatz solution. The crossover to strong coupling is a vestige of the phase transition into the broken-symmetry state. Landau parameters, charge and spin correlations of the heavy Fermi liquid are directly related to the fluctuations about the broken-symmetry state. The general approach presented is applicable to an arbitrary number of impurities or a lattice. Analytic results are presented for the Landau parameters, the dynamical charge and spin correlations in the one- and the two-impurity models, and the one-impurity f spectral function.

I. INTRODUCTION

The anomalous physical properties of heavy-fermion and mixed-valence systems at low temperatures raise many theoretical questions.[1-3] At the heart of the theoretical problem posed by these systems is the issue of how we should model their low-temperature, strong-coupling properties. There are two conceptual frameworks within which we are accustomed to treating these systems: the renormalization group and the Fermi-liquid picture.

In the language of the renormalization group the mixed-valence and Kondo systems are systems with spin and charge correlations spanning many decades of frequency, each decade contributing a logarithmic correction to the renormalized parameters such as the Kondo coupling constant $J(\Lambda)$, at lower frequencies. At the critical frequency scale of the Kondo temperature T_K the strength of interaction between the electrons becomes comparable with the electron kinetic energies, and at this point there is a crossover into strong coupling where the correlation effects of interactions can no longer be treated as a perturbation to electronic motions. To continue scaling of the Hamiltonian below the Kondo temperature, we are obliged to resort to numerical renormalization-group methods[4] or to attempt to solve the problem exactly[5] and in practical terms; this limits us to the single-impurity problem and to calculations of purely static correlations.

Nozières[6] recognized for the one-impurity Kondo problem that the low-temperature fixed point of the renormalization-group approach is a local Fermi liquid, and he deduced the low-temperature Fermi-liquid properties, such as the Wilson ratio $\tilde{x}/\tilde{\gamma}=(2j+1)/2j$ from purely Fermi-liquid arguments. It is generally accepted that concentrated heavy-fermion systems can be viewed as the Fermi-liquid "fixed point" of a model such as the Anderson lattice model. Unfortunately, if we wish to deduce Fermi-liquid properties which depend on the intersite coherence of the heavy Fermi liquid (such as the triplet interaction parameter), then we require more than Fermi-liquid phenomenology, for there are simply too many degrees of freedom to constrain the Landau parameters by using the Fermi-liquid arguments that are so powerful for one impurity.

High-temperature perturbation theories with careful renormalizations have been developed in attempts to enter the strong-coupling regime. One of the most successful of these techniques has been the large-N perturbation theories, where large spin degeneracy $N=2j+1$ is used to provide the expansion parameter $1/N$ for variational[7] or perturbation schemes.[8-12] Generally speaking, these approaches tackle the problem in a language most appropriate to weak coupling, expressing the dynamics in terms of correlation functions spanning many frequency decades, rather than expressing the low-energy physics in terms of a Fermi-liquid picture. Major difficulty is encountered upon attempting to extend these approaches beyond the one-impurity model, because the cluster expansions generated by the perturbation series do not naturally lend themselves to incorporation of multiple intersite scattering.

This paper presents a different conceptual framework which links the latter approaches. We will show that one can regard strong coupling in the Kondo effect *and* its many-site analogue, as an "almost broken symmetry:" a low-dimensional critical phenomenon involving long-time fluctuations at each magnetic site, but no critical fluctuations in space. The long-time fluctuations at each site are independent because of local conservation laws, and the resulting low dimensionality of the fluctuations prevents the development of a true broken symmetry.

We can motivate this point of view in the one-impurity model by using Fermi-liquid arguments. Consider the Coqblin-Schrieffer[13] model for local moments with

$N(=2j+1)$-fold spin degeneracy

$$\hat{\mathscr{H}}=\sum_{k,m} E(k)c_{km}^{\dagger}c_{km}-\frac{J}{N}\sigma^{\dagger}\sigma \ . \tag{1.1}$$

Here $\sigma=\sum_{k,m} f_m^{\dagger}c_{km}$ and $f_m^{\dagger}$ creates an f electron with spin component m. Let us consider the general case where there are Q f electrons in the localized f state. The action of $\sigma^{\dagger}\,|\,Q\rangle=|\,\psi\rangle$ on the ground state $|\,Q\rangle$ removes one f electron into the band, reducing Q by one. Since n_f is a conserved quantity, the final state remains permanently in a state with $Q-1$ f electrons. By using Nozières' Fermi-liquid picture, we know that the initial ground state scatters quasiparticles elastically, without changing their spins, and the elastic scattering is determined by a f-channel phase shift $\delta_f=\pi Q/N$, using Friedel's sum rule. The action of $\sigma^{\dagger}$ on $|\,Q\rangle$ transforms it into a new space of states where it relaxes to a final-state ground state that is described by an f-channel phase shift $\delta_f=\pi(Q-1)/N$. The situation is identical to x-ray absorption, where a change in the number of localized electrons induces a change in the local scattering phase shift. From the x-ray catastrophy[14] we know that the response of the system to the suddenly Modified scattering potential is governed by a power-law relaxation of the wave function $\langle\psi(0)\,|\,\psi(\tau)\rangle\sim\tau^{-\alpha-1}e^{-i\Delta E\tau}$ where α is the Nozières—de Dominicis x-ray exponent $\alpha=\sum_f(\Delta\delta_f/\pi)^2=1/N$ in this case, and ΔE is the difference between initial- and final-state ground-state energies. Since the long-time evolution of the final state is into a Fermi-liquid *ground state,* an identical power-law relaxation will occur in our example. Consequently, we deduce that at long times

$$\langle Q\,|\,\sigma(\tau)\sigma^{\dagger}(0)\,|\,Q\rangle\sim 1/\tau^{1/N}\quad(\tau\to\infty) \tag{1.2}$$

(where the oscillatory factor $e^{-i(E_{Q+1}-E_Q)\tau}$ due to the difference in ground-state energies has been omitted).

This infrared power-law correlation of operators that are off diagonal in the conserved quantity $\hat{Q}$ is a hallmark of strong coupling in the Kondo problem. In fact, from (1.2) we can deduce the asymptotic form of the renormalized Kondo coupling constant. When we integrate out the high-lying states of the Hillbert space in a renormalization treatment of the Kondo problem, we replace the instantaneous bare Kondo interaction by a time-dependent interaction with coupling constant given in weak coupling by

$$J^*(\tau)=J_0\delta(\tau)+J_0^2\langle Q\,|\,\sigma(\tau)\sigma^{\dagger}(0)\,|\,Q\rangle \ .$$

In strong coupling (low frequencies) the singular part of the coupling constant is given by

$$J^*(\omega)Z_f(\omega)\sim J_0^2\langle Q\,|\,\sigma(\tau)\sigma^{\dagger}(0)\,|\,Q\rangle_{\omega} \ ,$$

where $Z_f(\omega)=[(\partial/\partial\omega)G_f(\omega)^{-1}]^{-1}$ is the wave-function renormalization of the f electron. From Eq. (1.2), $Z_f(\omega)J^*(\omega)\sim\omega^{-(1-1/N)}$. By similar x-ray arguments, power-law behavior also occurs in the f Green's function

$$G_f(\tau)=\langle Tf_m(\tau)f^{\dagger}m(0)\rangle\sim\tau^{-1/N} \ ,$$

so that $G_f(\omega+\Delta E)\sim\omega^{(1/N-1)}$ and the f wave-function renormalization constant scales as $Z_f(\omega)=\omega^{1/N}$. Combining these results, gives us the strong-coupling behavior of the dimensionless coupling constant $J(\omega)\sim\omega^{-1}$, and the strong-coupling form for the β function is

$$\beta(J)=\frac{\partial J(\omega)}{\partial\ln\omega}=-J,\quad J\to\infty \tag{1.3}$$

as deduced by Nozières. This provides a link between the Fermi-liquid picture and the scaling picture of the Kondo impurity.

There is a close analogy between the off diagonal power-law correlations in *time* of the Kondo problem and critical fluctuations in *space* found in one-dimensional (1D) quantum systems. In condensed-matter physics a good example of this behavior is in the one-dimensional Heisenberg antiferromagnet,[15] which has a broken symmetry antiferromagnetic ground state in the limit of infinite spin S. At finite spin S, long-wavelength spin-wave fluctuations induce critical power-law decay of the spin-spin correlation function[16]

$$\langle\mathbf{S}_n\cdot\mathbf{S}_m\rangle\sim(-1)^{n-m}\,|\,n-m\,|^{-3/(2S+2)},\quad |\,n-m\,|\to\infty \ . \tag{1.4}$$

Thus, even in a finite degeneracy system, the critical fluctuations of the order parameter do not destroy the qualitative features of the broken-symmetry state that forms in the infinite S limit. In particular, the long-distance correlations are intrinsically antiferromagnetic, and the low-lying collective modes are similar to the broken-symmetry state. The picture of an almost antiferromagnetic ground state is very useful for this system, and this forms the basis of Anderson's semiclassical treatment of the Heisenberg spin chain.[15]

From this example one learns that by making an expansion about a broken-symmetry mean-field theory, the most singular behavior of the magnetic susceptibility at long wavelengths is incorporated into the theory. Similar ideas have been useful in the application of Bardeen-Cooper-Schrieffer (BCS) theory to heavy nuclei, where the particle pairing is treated as a broken-symmetry condensate.[17] Witten[18] has developed these ideas extensively in his study of the large-N expansion of the $(1+1)$-dimensional Gross-Neveu model, which is a relativistic analogue of the Kondo model. He shows that one can derive the power-law singularity characterizing the decay of the order parameter by analyzing the Gaussian fluctuations about the mean-field theory. Similar ideas are present in a somewhat different guise, in the theory of Kosterlitz and Thouless[19] for the 2D xy model.

These considerations strongly motivate us to regard the strong-coupling regime of the Kondo effect as a low-dimensional critical phenomenon with critical fluctuations in time about a state of almost broken symmetry. Within this picture, zero-mode fluctuations present in finite degeneracy systems restore the symmetry and generate the divergence of the Kondo coupling constant.

These arguments extend to many sites. Let us define $\sigma_{(j)}=\sum_{k,m} f_m^{\dagger(j)}c_{km}^{(j)}$ for each site j where $c_{km}^{\dagger(j)}$ creates a conduction electron in the same partial wave state as the f state. Conservation of Q_j at each site ensures

$\langle Q \mid \sigma_{(j)}(\tau)\sigma^{\dagger}_{(i)}(0) \mid Q \rangle = 0$ for $i \neq j$. For $i=j$, *provided* that a nonmagnetic Fermi liquid is formed where the local moments are fully quenched, the application of the operator $\sigma_{(j)}$ to the ground state creates a permanent hole with Q_j reduced by 1. The hole generates a persistent local scattering potential which induces power-law decay of the correlation function $\langle Q \mid \sigma_{(j)}(\tau)\sigma^{\dagger}_{(j)}(0) \mid Q \rangle$ as the state relaxes to the new ground state with a hole at site j. In the case of one impurity, local rotational invariance about the impurity guaranteed that there were N degenerate scattering phase shifts created by the hole. In the more general case the local scattering phase shifts will not all be degenerate (as we shall see for two impurities), and the x-ray exponent is $\alpha = \gamma/N$ where γ is of order one:

$$\langle Q \mid \sigma_i(\tau)\sigma^{\dagger}_j(0) \mid Q \rangle \sim \delta_{ij} 1/\tau^{\gamma/N}, \quad \tau \to \infty \ . \tag{1.5}$$

The most important point is that independent conservation of f charge at each site leads to critical fluctuations in time, but not in space.

The recognition that an underlying local symmetry can be associated with the strong local correlations governing heavy Fermi liquids is at the heart of this approach. In the case of the Coqblin-Schrieffer model, the f-electron number is the conserved quantity. In the more general case of mixed valence, charge fluctuations are restricted to a subspace of all possible f configurations, usually $\{f^n, f^{n+1}\}$, and the projection operator P into this subspace provides the conserved quantity associated with low-frequency charge fluctuations.

From a mathematical perspective, this philosophy evolves naturally from the pioneering functional-integral treatment of the Kondo problem proposed by Chakravarty[20] and developed extensively in the context of the large-N expansion by Read and Newns.[21] Within their formalism, the broken-symmetry state appears as the large-N saddle point.

A technical problem encountered in the early use of the functional-integral approach was caused by constraining Q to one, as in the conventional Kondo model. This caused difficulties, because intersite correlations then become a $1/N$ effect and vanish from the mean-field theory, and extensions to finite temperature or field become difficult.[22] True mean-field behavior occurs when $N \to \infty$ with $q = Q/N$ finite, thereby leading to "macroscopic" occupation of the f state. By preserving the full functional dependences in q in the $1/N$ expansion about the broken-symmetry state, intersite interactions are preserved and a useful $1/N$ expansion is developed.

This change in the way the large-N limit is taken makes it possible to extract mean-field behavior from the large-N limit of exact Bethe-ansatz equations for one impurity[23] as shown by Coleman and Andrei. They have solved the Coqblin-Schrieffer model and the analogous generalization of the infinite-U Anderson model for general Q, and demonstrated that when $N \to \infty$ with Q/N finite, the mean-field equations derived by direct means appear as the large-N limit of the Bethe-ansatz solutions.

It is illuminating to directly derive the properties of the broken-symmetry limit for the Coqblin-Schrieffer model. By inserting $\langle \sigma \rangle / \sqrt{N} = \tilde{\sigma}$ into (1.1), we arrive at the mean-field theory governing the large-N limit,

$$\mathscr{H}^{*} = \sum_{k,m} E(k) c^{\dagger}_{km} c_{km} + \tilde{V} \sum_{k,m} (c^{\dagger}_{km} f_m + \text{H.c.}) + E(\hat{Q} - Q_0) \ , \tag{1.6}$$

where $\tilde{V} = -J\tilde{\sigma}$ and we have associated a Lagrange multiplier of chemical potential E with the conserved quantity Q to aid in constraining it to the value Q_0.

This one-particle mean-field theory describes a resonance level at position E with width $\tilde{\Delta} = \pi \tilde{V}^2 \rho = (\pi J^2 \rho)\tilde{\sigma}^2$, where $\rho(\omega)$ is the density of states in the band, which we assume to be slowly varying on the scale of $\tilde{\Delta}$. The mean-field theory breaks the symmetry associated with Q conservation, and it only gives answers accurate to $O(1/N)$ due to the fluctuations $\langle \delta q^2 \rangle = O(1/N)$ present in the broken-symmetry state. In the real Coqblin-Schrieffer model we ultimately have to go beyond the mean-field treatment to incorporate fluctuations. We now use this mean-field Hamiltonian to self-consistently determine $\tilde{\sigma}$ and $q = \langle \hat{Q} \rangle / N$.

As $\mathscr{H}^{*}$ is a noninteracting Hamiltonian, it is very straightforward to calculate $\tilde{\sigma}$ and $q = \langle \hat{Q} \rangle / N$ directly using standard techniques. We find

$$\tilde{\sigma} = \tilde{V} \rho \, \text{Re} I(\xi) \ \text{ and } \ q = \text{Im} I(\xi) \ , \tag{1.7}$$

where $\xi = E + i\tilde{\Delta}$,

$$I(\xi) = \int \frac{d\varepsilon}{\pi} f(\varepsilon) \frac{\Phi(\varepsilon)}{\varepsilon - \xi} \ , \tag{1.8}$$

and $\Phi(\varepsilon) = \rho(\varepsilon)/\rho(\varepsilon_F)$ is the ratio of electronic density of states at ε to the value $\rho(\varepsilon)$ at the Fermi energy ε_F. In (1.7) we assume that the bandwidth D is much greater than $\tilde{\Delta}$. Employing a Lorentzian cutoff function $\Phi(\varepsilon) = D^2/(\varepsilon^2 + D^2)$, we find

$$I(\xi) = \frac{1}{\pi} \left[\psi \left(\frac{1}{2} + \frac{\xi\beta}{2\pi i} \right) - \ln \frac{D\beta}{2\pi i} \right] \tag{1.9}$$

where ψ is the digamma function, so that (1.7) can be written as one compact equation

$$\ln \frac{T_K}{2\pi T} + iq\pi = \psi \left(\frac{1}{2} + \frac{\xi\beta}{2\pi i} \right) + \frac{i\pi}{2} \ , \tag{1.10}$$

where

$$T_K = D e^{-1/J\rho} \tag{1.11}$$

is recognized as the leading order expression in the $1/N$ expansion Kondo temperature.[13,24,25] At $T=0$, $\psi(\beta z) \to \ln(z\beta)$ and (1.10) becomes

$$\ln \xi = \ln T_K + i\pi q \tag{1.12}$$

or

$$\xi = T_K e^{iq\pi} \ . \tag{1.13}$$

This expression demonstrates that the broken-symmetry state corresponds to a resonance level with $(E^2 + \tilde{\Delta}^2)^{1/2} = T_K$, whose position is tuned through the Fermi level by the value of the phase shift $\delta = \pi q$. This resonance level is naturally identified with the Abirikosov-Suhl resonance, and it is satisfying to discover

that this strong-coupling feature appears as naturally in this mean-field treatment. Chakravarty, Newns, and Read obtained this expression for the case when $q=1/N$ from the saddle point of their functional-integral formation.[20,21,26]

The paper is divided into four parts. The first section examines the mean-field theory in a variety of different cases, using the generalized Anderson model to extend this approach to mixed valence. The second section employs Newns's and Read's path-integral formalism to evaluate and relate the fluctuations about mean-field theory to the electronic correlations of strong coupling. Explicit calculations are presented for the one-impurity model, showing how the dynamic spin and charge susceptibilities, the Nozières Fermi-liquid parameters and the f-electron propagator can be evaluated in the one-loop or Gaussian approximation. Particular emphasis is laid on the way in which the fluctuations conserve q. The third section extends the approach to the two-impurity model, presenting analytic results for the Gaussian correlations, and emphasizing the new features which arise from a spatially extended, coherent Fermi liquid, such as exchange interactions and intersite spin correlations. In the final part, we discuss the extension of this formalism to a lattice, showing how the local constraints are consistently imposed in the Gaussian fluctuations and setting down the approach for a realistic angular momentum structure.

II. MEAN-FIELD THEORY

A. Generalized Anderson model

The infinite-U Anderson model has recently been generalized by the author in a way which exploits the underlying symmetry associated with restricting charge fluctuations to a few valence states.[22] "Slave-boson fields" b are introduced which describe the availability of an f state for hybridization. For the single impurity the generalized Anderson model is written

$$\mathscr{H}(\lambda)=\sum_{k,m}E(k)c^{\dagger}_{km}c_{km}+\sum_{m}E_f f^{\dagger}_m f_m+\mathscr{H}_{\rm mix}+\lambda(\hat{Q}-Q_0)\,, \tag{2.1}$$

where

$$\mathscr{H}_{\rm mix}=\frac{1}{\sqrt{N}}\sum_{k,m}V(k)(c^{\dagger}_{km}f_m b^{\dagger}+b f^{\dagger}_m c_{km}) \tag{2.2}$$

induces mixing between the localized f states and band electrons, while

$$\hat{Q}=\sum_m f^{\dagger}_m f_m+b^{\dagger}b \tag{2.3}$$

is a conserved charge which plays the analogous rôle to Q in the Coqblin-Schrieffer model. The sums over m run from $-j$ to j. The operator $c^{\dagger}_{km}$ creates a band electron in the partial wave state of energy $E(k)$ with the same total angular momentum numbers $|jm\rangle$ as an f state. $b^{\dagger}$ creates a local boson, and $b^{\dagger}$ satisfies canonical commutation laws $[b,b^{\dagger}]=1$.

In the case $Q=1$, the generalized Anderson model reverts to the infinite-U Anderson model, with the identification $b^{\dagger}|0\rangle=|f^0\rangle$ and $f^{\dagger}_m|0\rangle=|f^1{:}jm\rangle$. In fact, setting

$$\begin{aligned} &X_{00}=b^{\dagger}b,\quad X_{m'm}=f^{\dagger}_{m'}f_m\,,\\ &X_{0m}=b^{\dagger}f_m,\quad X_{m0}=f^{\dagger}_m b\,, \end{aligned} \tag{2.4}$$

we find that the $X_{\alpha\beta}$ obey the commutation algebras:

$$[X_{\alpha\beta},X_{\gamma\delta}]=\delta_{\beta\gamma}X_{\alpha\delta}-\delta_{\alpha\delta}X_{\gamma\beta}$$

which can be identified as the commutation algebra of the Hubbard operators introduced by Hubbard[27] for the infinite-U Anderson model, enabling us to write (2.1) in a more familiar form:

$$\begin{aligned} &\mathscr{H}=\sum_{k,m}E(k)c^{\dagger}_{km}c_{km}+(\lambda+E_f)\sum_m X_{mm}+\mathscr{H}_{\rm mix}+\lambda X_{00}\,,\\ &\mathscr{H}_{\rm mix}=\frac{1}{\sqrt{N}}\sum_{k,m}V(k)(c^{\dagger}_{km}X_{0m}+X_{m0}c_{km})\,, \end{aligned} \tag{2.5}$$

For the case $E_f\ll 0$ (taking the Fermi energy equal to 0), we can carry out a canonical transformation to integrate out the Bose field, in which case we arrive back at the Coqblin-Schrieffer model with $J=-V^2/E_f$ and $Q=n_f$.

When we extend this generalized model to many sites, or the lattice, we are able to interpret the slave-boson field as a smeared background hole density, or in analogy with liquid helium, as a collective backflow associated with the motion of the electrons. Since Q is conserved, the inflow of an f electron is always accompanied by a backflow of the Bose field. When the bose field has a small amplitude, the backflow is restricted and the f electrons become highly localized. The strong correlations of the f electrons are actually built into the model by the Q conservation symmetry. This is easily seen by noting that the matrix element

$$\langle f^{n+1};Q\,|\,\mathscr{H}_{\rm mix}\,|\,k;f^n\rangle=V(k)\sqrt{(Q-n)/N}\,, \tag{2.6}$$

showing that the absorption of a band electron into the f level depends on the occupation and becomes zero when $n_f=Q$. To constrain $\hat{Q}=Q_0$ in the thermodynamic ensemble, a Lagrange multiplier has been associated with Q.

So far as the mean-field theory of the generalized Anderson model is concerned, we can actually develop the equations governing the behavior of the broken-symmetry state at $N=\infty$ using straightforward operator quantum mechanics.

B. Mean-field behavior—single impurity

If we treat $\langle\hat{b}(t)\rangle/\sqrt{N}=\tilde{b}(t)$ as a c-number, as is appropriate in the $N\to\infty$ limit, we arrive at the mean-field Hamiltonian governing the motion of the electron for one impurity

$$\mathscr{H}^{*}(t)=\sum_{k,m}E(k)c^{\dagger}_{km}c_{km}+\sum_m\tilde{E}_f f^{\dagger}_m f_m+\hat{\mathscr{H}}_{\rm mix}(t)\,, \tag{2.7}$$

where

$$\hat{\mathscr{H}}_{\rm mix}(t)=\sum_{k,m}\frac{V(k)}{\sqrt{N}}[c^{\dagger}_{km}f_m b^{*}(t)+f^{\dagger}_m c_{km}b(t)]\,. \tag{2.8}$$

The dynamics of the Bose field are determined from the equation of motion $i\partial\tilde{b}/\partial t=\langle[\mathscr{H},\tilde{b}(t)]\rangle$, or

$$-\frac{i\partial\tilde{b}}{\partial t}=\lambda\tilde{b}(t)+\frac{1}{N}\sum_{k,m}V(k)\langle c^{\dagger}_{km}(t)f_m(t)\rangle \tag{2.9}$$

plus the constraint

$$q_0=|\tilde{b}(t)|^2+\tilde{n}_f(t)\ , \tag{2.10}$$

where $\tilde{n}_f=\langle\hat{n}_f\rangle/N$. Equations (2.7) to (2.10) completely describe the mean-field behavior occurring in the large-N limit. We see that the Bose field acts as a dynamic potential field which governs the mixing of the band and f electrons.

To go beyond mean field requires a perturbation theory about the coherent states of definite b and the path-integral formalism becomes useful at this point. For the moment we shall confine ourselves to a brief discussion of how the equations of motion (2.7) to (2.10) arise as saddle points of this path-integral formalism.

C. Mean-field behavior from path-integral formalism: single impurity

The partition function of the Gibbs ensemble with definite $Q=Q_0$ is written[26,22]

$$Z(Q_0)=\int_0^{2\pi i/\beta}\frac{\beta d\lambda}{2\pi i}Z(\lambda)e^{\beta\lambda Q_0}\ , \tag{2.11}$$

where $\beta=1/k_BT$ and

$$Z(\lambda)=\mathrm{Tr}e^{-\beta\hat{\mathscr{H}}[\lambda]}\ . \tag{2.12}$$

In (2.11) the Fourier transform over the Lagrange multiplier λ constrains $Q=Q_0$. $Z(\lambda)$ can be written as a path integral over the Bose and Fermi fields

$$Z(\lambda)=\int\mathscr{D}[\bar{\psi},\psi]\mathscr{D}[\bar{b},b]e^{-\beta F[\psi,\bar{\psi};\bar{b},b]}\ , \tag{2.13}$$

where

$$\beta F[\bar{\psi},\psi;\bar{b},b]=\int_0^{\beta}d\tau\left[\sum_i\bar{\psi}_i(\tau)\frac{\partial}{\partial\tau}\psi_i+\bar{b}(\tau)\frac{\partial}{\partial\tau}b(\tau)+\mathscr{H}[\lambda]\right] \tag{2.14}$$

is the full free-energy functional. Here $\bar{\psi}_i$ and ψ_i denote the Fermi fields (formally represented by Grassman variables) and $\bar{b},b$ are the c-numbers representing the Bose field and its complex conjugate. $\mathscr{D}[\bar{\psi},\psi]$ and $\mathscr{D}[\bar{b},b]$ are standard Cartesian measures for Fermi and Bose path integrals. τ is the imaginary time variable and implicit in the functional integral are periodic boundary conditions for the Bose fields and antiperiodic boundary conditions for the Fermi fields, $\psi(\tau+\beta)=-\psi(\tau)$ and $b(\tau+\beta)=b(\tau)$.

To determine the saddle-point equations, we freeze the Bose field at each point in time and calculate the motion of the fermions in this external field. The path integral is then written as

$$Z(\lambda)=\int\mathscr{D}[\bar{b},b]\exp(-\beta F_{\mathrm{eff}}[\bar{b},b])\ , \tag{2.15}$$

where

$$\exp(-\beta F_{\mathrm{eff}}[\bar{b},b])=\int\mathscr{D}[\bar{\psi},\psi]\exp(-\beta F[\bar{\psi},\psi;\bar{b},b])\ . \tag{2.16}$$

F_{eff} is the effective free-energy functional for the Bose fields with the fermions integrated out of the dynamics. Since this integral is quadratic in the Fermi field, we can evaluate it to gain

$$\beta F_{\mathrm{eff}}[\bar{b},b]=\int_0^{\beta}d\tau\,\bar{b}(\tau)\left[\frac{\partial}{\partial\tau}+\lambda\right]b(\tau)+\beta F_{\psi}[\bar{b},b]\ , \tag{2.17}$$

where $F_{\psi}[\bar{b},b]$ is the fermion free energy for the frozen Bose field configuration $b(\tau)$.

This is expressed compactly as a trace over the Fermion field space and imaginary time

$$\beta F_{\psi}[\bar{b},b]=-\mathrm{Tr}_{\bar{\psi},\psi}\ln\left[\hat{1}\frac{\partial}{\partial\tau}+\hat{\mathscr{H}}^*[\bar{b},b]\right]\ , \tag{2.18}$$

where $\hat{\mathscr{H}}^*[\bar{b},b]=\hat{\mathscr{H}}^*(\tau)\delta(\tau-\tau')$ and $\hat{\mathscr{H}}^*(\tau)$ is the time-dependent Hamiltonian of (2.7). The trace in (2.18) involves a trace over imaginary time and the full Fock space of the fermions, i.e.,

$$\mathrm{Tr}_{\bar{\psi},\psi}\hat{A}=\int_0^{\beta}d\tau\,\mathrm{Tr}_{\bar{\psi},\psi}\hat{A}(\tau,\tau) \tag{2.19}$$

and $(\bar{\psi},\psi)$ denotes the trace over the Fock space. The full partition function (2.11) can now be written

$$Z(Q_0)=\int_0^{2\pi i/\beta}\frac{\beta d\lambda}{2\pi i}\times\int\mathscr{D}[\bar{b},b]\exp\{-\beta(F_{\mathrm{eff}}[\bar{b},b]-\lambda Q_0)\}\ . \tag{2.20}$$

If we take $N\to\infty$ with $Q_0/N=q_0$ finite, then the exponent of this path integral becomes extensive in N, allowing us to approximate $Z(Q_0)$ by its saddle-point value

$$Z(Q_0)=\exp(-\beta\{F_{\mathrm{eff}}[\bar{b}(\tau),b(\tau)]-\lambda_0Q_0\})\ , \tag{2.21}$$

where $b(\tau)$, λ are the saddle points of $\Omega_{\mathrm{eff}}=F_{\mathrm{eff}}+\lambda Q_0$. Directly taking the derivatives of (2.16), we find

$$\frac{\delta\Omega_{\mathrm{eff}}}{\delta\bar{b}(\tau)}=\left[\frac{\partial}{\partial\tau}+\lambda_0\right]b(\tau)+\frac{1}{\sqrt{N}}\sum_{k,m}V(k)\langle c^{\dagger}_{km}(\tau)f_m(\tau)\rangle=0\ , \tag{2.22}$$

$$\frac{\delta\Omega_{\mathrm{eff}}}{\partial\lambda}=|b(\tau)|^2+\langle\hat{n}_f\rangle-Q_0=0\ ,$$

which are Eqs. (2.9) and (2.10) expressed in imaginary time $\tau=it$.

D. Mean field in thermal equilibrium: Phase diagram for strong coupling

In thermal equilibrium we apply a static solution to the Bose field $\langle\hat{b}\rangle/\sqrt{N}=\tilde{b}=\mathrm{const}$, from which we gain

$$\lambda_0\tilde{b}+\frac{1}{N}\sum_{k,m}V(k)\langle c^{\dagger}_{km}f_m\rangle_{\tilde{b}=\mathrm{const}}=0, \tag{2.23}$$

$$\tilde{r}^2+\tilde{n}_f=q_0,$$

where $q_0=Q_0/N$ and $\tilde{r}=|\tilde{b}|$.

The expectation values in these equations are then determined self-consistently using the Hamiltonian (2.7) with a constant $\tilde{b}(\tau)=\tilde{b}=\tilde{r}_0 e^{i\theta}$. This is a very straightforward task, as (2.7) is now a static one-particle Hamiltonian. The one-particle Green's functions

$$\sum_k V(k)\langle Tf_m(\tau)c_{km}^\dagger(0)\rangle = G_{fk}(\tau)$$

and

$$\langle Tf_m(\tau)f_m^\dagger(0)\rangle = G_f(\tau)$$

are given by

$$\begin{aligned} G_f(i\omega_n)&=[i\omega_n-\tilde{E}_f-\tilde{r}_0^2\Sigma_f(i\omega_n)]^{-1}\ , \\ G_{fk}(i\omega_n)&=\tilde{r}_0\Sigma_f(i\omega_n)G_f(i\omega_n)\ , \end{aligned} \tag{2.24}$$

where the Green's functions are Fourier transformed with the convention that

$$G_\alpha(\tau)=-\beta^{-1}\sum_n G_\alpha(i\omega_n)e^{-i\omega_n\tau}\ ,$$

and

$$\Sigma_f(i\omega_n)=\sum_k |V(k)|^2/[i\omega_n-E(k)]\ . \tag{2.25}$$

For a large symmetric band of width D, where $V(k)$ and the density of states in the band are assumed to vary smoothly over the scale of energies characterizing the low-energy quasiparticle excitations, the analytic extension of $\Sigma_f(i\omega_n)$ is given by

$$\Sigma_f(\omega)=-i\,\mathrm{sgn}(\omega_I)\Delta\tilde{r}_0^2\Phi(\omega)+O(\omega/D,\Delta/D)\ , \tag{2.26}$$

where $\omega_I=\mathrm{Im}\omega$, $\Delta=\pi\rho|V(k_F)|^2$ is the bare resonance level width and ρ is the density of states at the Fermi energy. $\Phi(\omega)=\rho(\omega)/\rho$ defines the variation of the band density of states away from the Fermi energy. This approximation is of course only appropriate for the low-energy, long-time behavior $\tau\gg D^{-1}$. Now we can relate

$$\begin{aligned} \frac{1}{N}\sum_{k,m} V(k)\langle c_{km}^\dagger f_m\rangle &= \beta^{-1}\sum_n G_{fk}(i\omega_n)e^{i\omega_n 0^+}\ , \\ \frac{1}{N}\sum_m \langle f_m^\dagger f_m\rangle &= \beta^{-1}\sum_n G_f(i\omega_n)e^{i\omega_n 0^+}\ . \end{aligned} \tag{2.27}$$

Carrying out these integrals by conventional contour integrations, and deforming the contour about the cut along the real axis generated by $\Sigma_f(z)$, in a similar calculation to (1.8) we find

$$\begin{aligned} \frac{1}{N}\sum_{k,m} V(k)\langle c_{km}^\dagger f_m\rangle &= \frac{\Delta\tilde{b}}{\pi}\,\mathrm{Re}I(\tilde{E}_f+i\tilde{\Delta})\ , \\ \frac{1}{N}\sum_m \langle f_m^\dagger f_m\rangle &= \mathrm{Im}I(\tilde{E}_f+i\tilde{\Delta})\ , \end{aligned} \tag{2.28}$$

where $\tilde{\Delta}=\Delta\tilde{r}_0^2$ is a renormalized resonance level width characterizing the mean-field resonant f level as in (1.8). Using the result (1.9) for a Lorentzian cutoff $\Phi(\omega)=D^2/(\omega^2+D^2)$, we find that we can write (2.22) as one equation,

$$\frac{\Delta}{\pi}\left[\tilde{\psi}(\xi)-\mathrm{Im}\frac{\Delta\beta}{2\pi^2 i}\right]+\xi=E_f^*+i\Delta q\ . \tag{2.29}$$

Here we have introduced the complex f-level position

$$\xi=\tilde{E}_f+i\tilde{\Delta}=(E_f+\lambda)+i\Delta\tilde{r}_0^2 \tag{2.30}$$

and denoted

$$\tilde{\psi}(\xi)=\psi\left[\frac{1}{2}+\frac{\xi\beta}{2\pi i}\right]\ . \tag{2.31}$$

The quantity

$$E_f^*=E_f+\frac{\Delta}{\pi}\ln\left[\frac{D\pi}{\Delta}\right] \tag{2.32}$$

contains all the cutoff dependence in the mean-field theory, and it is recognized as the leading order $O(1/N)$ expression for the Haldane invariant f level[28,29]

$$E_f^*(N)=E_f+\frac{\Delta}{\pi}\left[1-\frac{1}{N}\right]\ln\left[\frac{D\pi}{\Delta}\right] \tag{2.33}$$

which characterizes the high-frequency charge fluctuations.

If we let $T\to 0$, (2.28) reverts to the form

$$\frac{\Delta}{\pi}\ln\left[\frac{\xi\pi}{\Delta}\right]+\xi=E_f^*+i\Delta q\ . \tag{2.34}$$

In the Kondo limit $|\xi|\ll\Delta$ and the logarithm (or digamma) function dominates the mean-field behavior. By setting $J\rho=-\Delta/E_f$, we arrive back at the mean-field expression for the Coqblin-Schrieffer model derived in the Introduction (1.10). It is remarkable that the introduction of charge fluctuations into the mean-field theory produces such a simple modification to the saddle-point equations. Read and Newns[26] first obtained (2.34) for the case $q=1/N$.

Equation (2.29) can be solved self-consistently for ξ. Sample curves for $\tilde{r}_0^2=(\tilde{\Delta}/\Delta)$ are shown in Fig. 1. The renormalized width $\tilde{\Delta}$ vanishes at $T=T_c$ given by

$$\begin{aligned} \xi&=2T_c\tanh^{-1}(1-2q)\ , \\ \frac{2T_c\pi}{\Delta}\tanh^{-1}(1-2q)&+\mathrm{Re}\psi\left[\frac{1}{2}+\frac{\tanh^{-1}(1-2q)}{\pi i}\right] \\ &=\frac{\pi E_f^*}{\Delta}+iq\pi\ . \end{aligned} \tag{2.35}$$

At $T>T_c$ the mean-field solution becomes the trivial solution $b=0$, $f(\xi)=q$ corresponding to unquenched localized f electrons.

These expressions can all be modified to incorporate an interaction with a magnetic field

$$\mathscr{H}_B=-Bg\mu_B\sum_m m\hat{n}_{fm}\ . \tag{2.36}$$

Placing $h/N=g\mu_B B$, we find on reevaluating $\langle c_{km}^\dagger f_m\rangle$

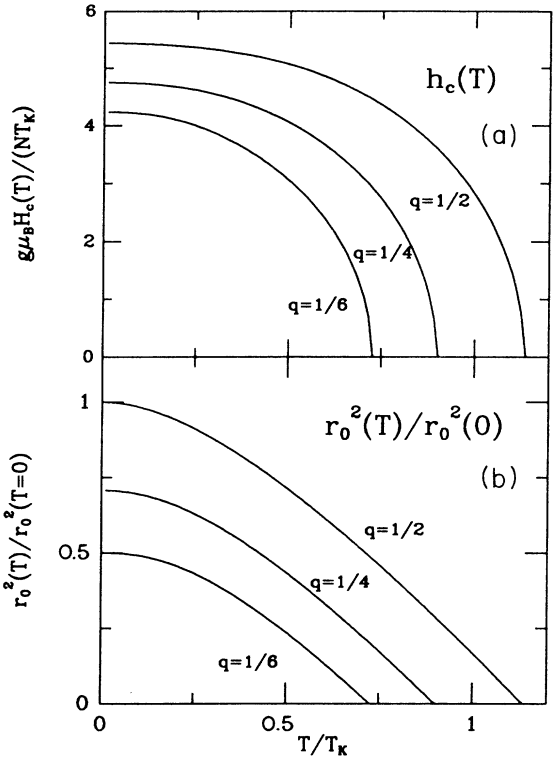

FIG. 1. (a) The mean-field phase boundary $h_c(T)$ separating strong from weak coupling in the one-impurity model for various filling factors. (b) Variation of $\tilde{r}_0^2(T)=\tilde{\Delta}(T)/\Delta$ in the mean-field theory.

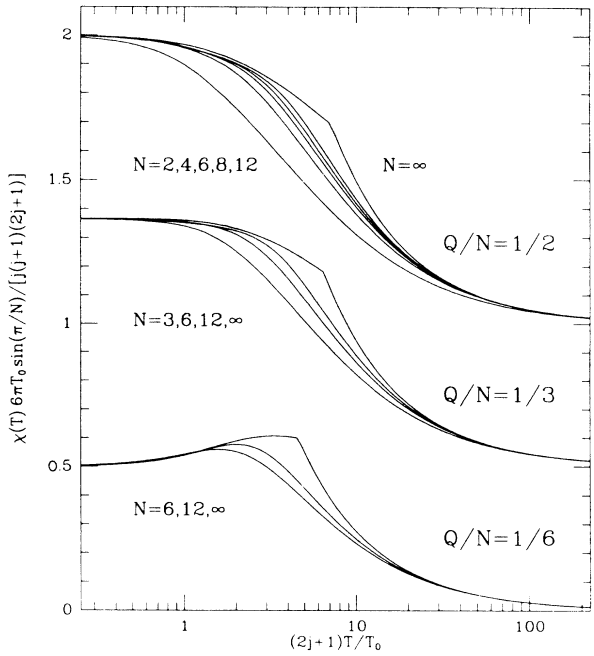

FIG. 2. Comparison of Bethe-ansatz results with mean-field theory, displaying the susceptibility $\tilde{\chi}(T)2\pi T_0\sin(\pi/N)=\chi(T)6\pi T_0\sin(\pi/N)/[j(j+1)(2j+1)]$ for the sequences $Q/N=\frac{1}{2}$, $\frac{1}{3}$, $\frac{1}{6}$, where at $T=0$, in the Kondo regime $\tilde{\chi}(T=0)2\pi T_0\sin(\pi/N)=\sin(\pi Q/N)$. The curves for $Q/N=1/2$ and $Q/N=\frac{1}{3}$ are shifted upwards by 0.5 and 1.0 units, respectively.

and $\langle\hat{n}_f\rangle$ that the mean-field equations become

$$\xi+\frac{\Delta}{\pi}\left[\sum_{m=-j}^{j}\frac{1}{N}\tilde{\psi}\left[\xi+\frac{m}{N}h\right]-\ln\left[\frac{\Delta\beta}{2\pi i}\right]\right]=E_f^*+i\Delta q\ , \tag{2.37}$$

where the sum over m corresponds to the $2j+1$ nondegenerate f levels. In the large-N limit we can replace the sum by an integral to find

$$\xi+\frac{\Delta}{\pi}\left[\frac{2\pi i k_B T}{h}\right]\ln\left[\frac{\tilde{\Gamma}(\xi+h/2)}{\tilde{\Gamma}(\xi+h/2)}\right]-\frac{\Delta}{\pi}\ln\left[\frac{\Delta\beta}{2\pi^2 i}\right]=E_f^*+i\Delta q\ , \tag{2.38}$$

where

$$\tilde{\Gamma}(z)=\frac{1}{\sqrt{2\pi}}\Gamma\left[\frac{1}{2}+\frac{z\beta}{2\pi i}\right] \tag{2.39}$$

and $\Gamma(z)$ is the gamma function. The phase transition between strong and weak coupling is field dependent, occurring at $T_c(h)$ as shown in Fig. 1.

E. Comparison with Bethe ansatz

Coleman and Andrei[23] have calculated the f occupation of the single-impurity model using a Bethe-ansatz solution, and have explicitly taken the $N\to\infty$ limit with finite q. At $T=0$, $B=0$ they find

$$\frac{n_f}{N}=q_0-\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{1}{(\omega+i\delta)}[(-i\omega)^{-i\omega-1}\Gamma(1+i\omega)]\times e^{-i\omega(\pi E_f^*/\Delta)}\sinh(\pi\omega q) \tag{2.40}$$

and show that the right-hand term is nothing but the inversion of the mean-field equations for $\tilde{b}^2(E_f^*+i\Delta q)$. At finite degeneracy they find that

$$\frac{n_f}{N}=q_0-\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{-i(\omega+i\delta)}F(\omega)\frac{\sinh(\pi Q\omega/N)}{N\sinh(\pi\omega/N)}\times e^{-i\omega(\pi E_f^*/\Delta)}\ , \tag{2.41}$$

where the function $F(\omega)$ is given by

$$F(\omega)=\frac{\Gamma(1+i\omega)}{\Gamma(1+i\omega/N)}[-i(\omega-i\delta)]^{-i\omega(1-1/N)}e^{-|\omega|\pi/N}\ , \tag{2.42}$$

and $E_f^*=E_f+(1-1/N)(\Delta/\pi)\ln(D\pi/\Delta)$. An important feature of (2.41) is that it has a *perturbative* Taylor-series expansion in $1/N$ about the $N\to\infty$ limit (2.40). A similar agreement is obtained with the zero-temperature linear specific-heat coefficient and the zero-temperature magnetic susceptibility. At finite magnetic field, in the limiting case of the Coqblin-Schrieffer model, they are able to show that the mean-field result can be used as a precise solution to the Bethe-ansatz integral equations in the large-N limit. At finite T, the Bethe-ansatz equations

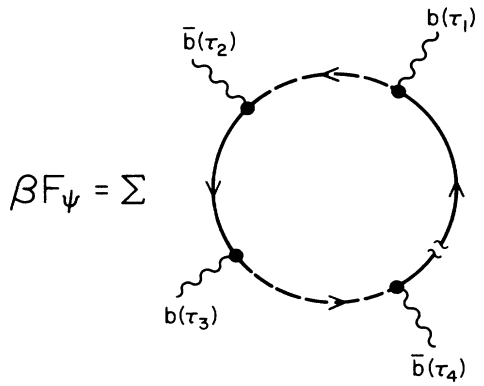

FIG. 3. Diagrammatic representation of the fermion loops entering into the boson free-energy functional. The dashed lines are unhybridized f propagators and the solid lines are conduction electron propagators.

have been solved numerically, for the case of the Coqblin-Schrieffer mode, and they show clearly the development of mean-field behavior as $N\rightarrow\infty$ with q fixed (Fig. 2). We may therefore be confident in the case of the single impurity, that the mean-field solution represents a smooth limiting case of the finite degeneracy solutions.

F. Thermodynamics

The direct calculation of the mean-field free energy $\Omega_{\rm MF}=\Omega_{\rm eff}(\tilde{b}_0,\lambda_0)$ enables us to generate the mean field of the large N limit, and in later sections this is employed to calculate the renormalizations that arise from the fluctuations.

From (2.17) we have

$$\Omega_{\rm MF}=N(\tilde{r}_0^2-q_0)\lambda+F_\psi(\tilde{b}=\tilde{r}_0)\ . \tag{2.43}$$

The fermion contribution to the free energy F_ψ can be written down compactly in terms of the f and band-electron propagators, enabling us to understand $F_\psi[\bar{b},b]$ diagrammatically.

To do this, let us define operators corresponding to the bare f and band-electron propagators

$$\hat{G}_{\rm band}=\left[\frac{\partial}{\partial\tau}+\mathscr{H}_{\rm band}\right]^{-1}=\sum_{k,m}c_{km}^\dagger(\tau)G_k(\tau-\tau')c_{km}(\tau')\ , \tag{2.44}$$

$$\hat{G}_f^{\,0}=\left[\frac{\partial}{\partial\tau}+\hat{\mathscr{H}}_f\right]^{-1}=\sum_m f_m^\dagger(\tau)G_f^{(0)}(\tau-\tau')f_m(\tau')\ . \tag{2.45}$$

Here the Fermi operators are in the Heisenberg representation, and the explicit expressions for $G_k(\tau)$ and $G_f^{(0)}(\tau)$ are

$$G_k(\tau)=-\beta^{-1}\sum_{i\omega_n}G_k(i\omega_n)e^{-i\omega_n\tau}$$

and

$$G_f^{(0)}(\tau)=-\beta^{-1}\sum_{i\omega_n}G_f^{(0)}(i\omega_n)\ ,$$

where

$$\begin{aligned}G_k(i\omega_n)&=[i\omega_n-E(k)]^{-1}\ ,\\ G_f^{(0)}(i\omega_n)&=(i\omega_n-\tilde{E}_f)^{-1}\ .\end{aligned} \tag{2.46}$$

Now if further we define the mixing operator

$$\hat{V}=b(\tau)\sum_{k,m}\frac{V(k)}{\sqrt{N}}c_{km}^\dagger(\tau)f_m(\tau)\ , \tag{2.47}$$

where $b(\tau)$ is a c-number, then we can compactly write the operator

$$\hat{1}\frac{\partial}{\partial\tau}+\hat{H}^*=\begin{bmatrix}\hat{G}_f^{(0)-1} & V^\dagger\\ V & \hat{G}_{\rm band}^{-1}\end{bmatrix}\ . \tag{2.48}$$

By using the identity

$$\mathrm{Tr}\ln\begin{bmatrix}A & C^\dagger\\ C & B\end{bmatrix}=\mathrm{Tr}\ln B+\mathrm{Tr}\ln(A-CB^{-1}C^\dagger)\ , \tag{2.49}$$

we are able to split F_ψ into a band-electron and f-electron contribution

$$F_\psi=F_{\rm band}-k_BT\,\mathrm{Tr}\ln\hat{G}_f^{-1}\ , \tag{2.50}$$

where $F_{\rm band}=-k_BT\,\mathrm{Tr}\ln\hat{G}_{\rm band}^{-1}$ is the constant band-electron contribution to F_ψ (henceforth omitted) and $\hat{G}_f$ is the full f-electron propagator in the presence of the Bose field, given by

$$\hat{G}_f^{-1}=\hat{G}_f^{(0)-1}-\hat{V}\hat{G}_{\rm band}\hat{V}\ . \tag{2.51}$$

We can write the propagator $G_f(\tau,\tau')$ as

$$G_f(\tau,\tau')=\{[G_f^{(0)}(\tau-\tau')]^{-1}+\tilde{\Sigma}_f(\tau,\tau')\}^{-1}\ , \tag{2.52}$$

where

$$\tilde{\Sigma}_f(\tau,\tau')=\frac{1}{N}b(\tau)\Sigma_f(\tau-\tau')\bar{b}(\tau') \tag{2.53}$$

is the f-electron self-energy in the dynamic Bose field and

$$\Sigma_f(\tau)=-\beta^{-1}\sum_n\Sigma_f(i\omega_n)e^{-i\omega_n\tau}$$

was defined in (2.25).

The f-electron free energy (with $F_{\rm band}$ omitted) can formally be written as a perturbation series in $\hat{V}$

$$\begin{aligned}F_\psi[b,\bar{b}]&=-k_BT\,\mathrm{Tr}\ln(\hat{G}_f^{(0)-1}+\tilde{\Sigma}_f)\\ &=-k_BT\,\mathrm{Tr}\ln\hat{G}^{(0)-1}\\ &\quad-k_BT\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}[(-\tilde{\Sigma}_f\hat{G}_f)^n]\ ,\end{aligned} \tag{2.54}$$

which we recognize as a sum of all closed-loop diagrams generated by contacting the f-and band-electron propagators in the presence of the dynamic Bose field (Fig. 3).

We will return to this general expression in the next

section. For the moment, by setting $b(\tau)/\sqrt{N}=\text{const}=\tilde{r}_0$, the f propagator reverts to the form shown in Eq. (2.24), allowing us to write

$$F_\psi^{\rm MF}=-Nk_BT\sum_{i\omega_n}\ln[\tilde{E}_f+\tilde{r}_0^2\Sigma_f(i\omega_n)-i\omega_n]\ , \quad (2.55)$$

where the prefactor arises from the sum over the $2j+1$ spins. Converting (2.50) into a contour integral and distorting it around the real axis gives

$$F_\psi=-N\int\frac{d\omega}{\pi}f(\omega)\phi(\omega)\delta(\omega)\ . \quad (2.56)$$

Here,

$$\delta(\omega)=\tan^{-1}\left[\frac{\tilde{\Delta}}{\tilde{E}_f-\omega}\right] \quad (2.57)$$

is the f-channel phase shift produced by the renormalized resonant level and $\phi(\omega)$ is the cutoff function $\phi(\omega)=D^2/(\omega^2+D^2)$. We will write

$$\begin{aligned}F_\psi&=-N\,\mathrm{Im}\int_{-\infty}^{+\infty}\frac{f(\omega)\phi(\omega)}{\pi}\ln(\xi-\omega)d\omega\\&=+\frac{N}{\pi}\,\mathrm{Im}\int_{-\infty}^{\xi}I(z)dz\end{aligned} \quad (2.58)$$

by (1.8). Thus by (1.9)

$$F_\psi=\frac{N}{\pi}\,\mathrm{Im}\left[2\pi ik_BT\ln\tilde{\Gamma}(\xi)-\xi\ln\frac{D\beta}{2\pi i}\right], \quad (2.59)$$

where $\tilde{\Gamma}(z)$ was defined in (2.39). When we add on $N(\tilde{r}_0^2-q_0)\lambda$ this gives

$$\Omega_{\rm MF}=N\,\mathrm{Im}\Omega_c^{\rm MF}\ , \quad (2.60)$$

where

$$\Omega_c^{\rm MF}=\frac{(\xi-E_c^*)^2}{2\Delta}+\left[2\pi ik_BT\ln\tilde{\Gamma}(\xi)-\frac{\xi}{\pi}\ln\frac{\Delta\beta}{2\pi i}\right] \quad (2.61)$$

and $E_c^*=E_f^*+i\Delta q_0$. In a finite field we can generalize this expression to

$$\Omega_c=\frac{(\xi-E_c^*)^2}{2\Delta}+\sum_m\left[\frac{2ik_BT}{N}\ln\tilde{\Gamma}(\xi_m)\right]-\frac{\xi}{\pi}\ln\frac{\Delta\beta}{2\pi i}\ , \quad (2.62)$$

where $\xi_m=\xi-(m/N)h=\xi-mg\mu_BB$.

From Ω_c we can quickly rederive the saddle-point equations from the stationary condition $\partial F/\partial\xi=0$. We can derive the f occupation in the mth channel from

$$n_{fm}=\left.\frac{\partial\Omega_{\rm MF}}{\partial\xi_m}\right|_{\xi,E_c^*}=\frac{1}{\pi}\,\mathrm{Im}\left[\tilde{\psi}(\xi_m)+\frac{i\pi}{2}\right]. \quad (2.63)$$

Thus, in small fields the magnetization is

$$M=\sum_m(g\mu_B)mn_{fm}=B[\tfrac{1}{3}(g\mu_B)^2j(j+1)(2j+1)]\tilde{\chi}_s\ , \quad (2.64)$$

where

$$\tilde{\chi}_s=-\,\mathrm{Im}[\tilde{\psi}'(\xi)/\pi]\ , \quad (2.65)$$

where $\tilde{\psi}'(\xi)=\partial\tilde{\psi}(\xi)/\partial\xi$. This result extrapolates smoothly from the result of Read and Newns at $T=0$

$$\tilde{\chi}_s=-\frac{1}{\pi}\,\mathrm{Im}\frac{1}{\xi}=\frac{1}{\pi}\frac{\tilde{\Delta}}{(\tilde{\Delta}^2+\tilde{E}_f^2)},\quad T=0 \quad (2.66)$$

to the weak-coupling value

$$\tilde{\chi}_s=q(1-q)/k_BT,\quad T>T_c\ . \quad (2.67)$$

It is this function that was used to calculate the large-N limit in Fig. 3. Similarly, the charge susceptibility is given by

$$\chi_c=-\frac{\partial n_f}{\partial E_f^*}=\frac{N}{\Delta}\,\mathrm{Im}\left[\left[1+\frac{\Delta}{\pi}\tilde{\psi}'(\xi)\right]^{-1}\right], \quad (2.68)$$

which extrapolates smoothly from the Read and Newns result at $T=0$,

$$\chi_c=\frac{N}{\Delta}\,\mathrm{Im}\left[\left[\frac{\Delta}{\pi\xi}+1\right]^{-1}\right], \quad (2.69)$$

to zero at high temperatures ($T>T_c$).

These results will be modified when we take into account the fluctuations. From these results, we see that the broken-symmetry state corresponds to a quenched local moment, whereas the weak-coupling regime with $b=0$ corresponds to free local moments. As a final indication of this result, we can calculate the entropy of the system, given by

$$\begin{aligned}S&=-\left.\frac{\partial\Omega}{\partial T}\right|_{\partial\Omega_c/\partial\xi=0}=-\,\mathrm{Im}\left.\frac{\partial\Omega_c}{\partial T}\right|_\xi\\&=-Nk_B\,\mathrm{Im}\{2i\ln\tilde{\Gamma}(\xi)+\xi\beta[\tilde{\psi}(\xi)-1]\}\ ,\end{aligned} \quad (2.70)$$

which extrapolates between the low-temperature limit[26]

$$S=N\tilde{\gamma}\frac{k_B^2}{3}\pi^2T \quad (2.71)$$

with $\tilde{\gamma}=\tilde{\chi}_s$ ($T=0$) and the high-temperature limit

$$S=-Nk_B[q\ln q+(1-q)\ln(1-q)] \quad (2.72)$$

corresponding to a proportion q of full f states, and a proportion $(1-q)$ of empty f states.

As we might expect, the mean-field thermodynamics are a poor approximation to the high-temperature thermodynamics of the finite degeneracy system, where fluctuations produce the all-important logarithmic tails in susceptibilities, leading to nontrivial high-temperature corrections. However, in the strong-coupling regime this simplistic approximation is qualitatively good and sums the most important logarithmic contributions in the interactions. Figure 4 shows plots of $C_V/T=dS/dT$ derived from (2.70).

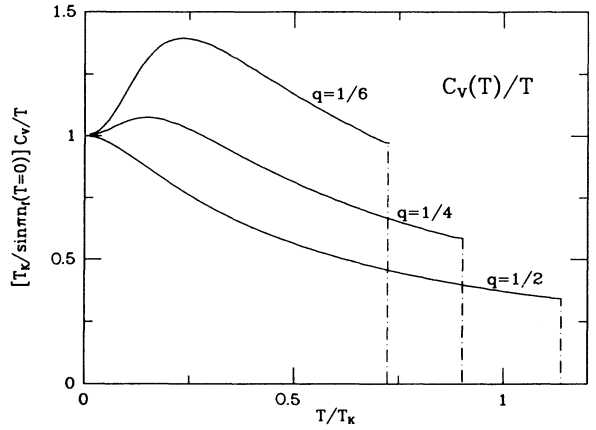

FIG. 4. Showing $\{T_K/\sin[\pi n_f(T=0)]\}C_V/T$, where $T_K=(\tilde{E}_f^2+\tilde{\Delta}^2)^{1/2}$. The plots are for the Kondo limit with $n_f/Q=0.95$, and they exhibit marked dependence on filling factor q.

G. Many sites

The generalized Anderson model can be written down for many impurities, or the lattice, by introducing a conserved charge Q_i for each site at position $\mathbf{R}_i$. Associated with each site is an auxiliary-boson ("slave-boson") field b_i describing the availability of site i for hybridization. One of the complicating problems associated with a real mixed-valence lattice is the angular momentum structure of the band and f electrons. In a real electron band the electrons have spin half, whereas the f electrons in a typical mixed valence are spin-orbit coupled into a state of definite j. Even excluding the effect of crystalline electric fields, which split the $(2J+1)$-fold degeneracy into smaller multiplets, this means that hybridization at each site occurs through those partial wave states with the same angular momentum quantum numbers as the spin-orbit-coupled f state. To describe this hybridization we need to project the band-electron states onto the appropriate local partial wave states. This is compactly accomplished with the overcomplete set of field operators for the band electrons

$$c_{km}^{\dagger}(\mathbf{R})=\sum_{\sigma=\pm 1/2}\int\frac{d\Omega_{\hat{\mathbf{k}}}}{4\pi}e^{-i\mathbf{k}\cdot\mathbf{R}}C_{jl\,1/2}^{m;m-\sigma}Y_{l,m-\sigma}^{*}(\hat{\mathbf{k}})c_{\mathbf{k}\sigma}^{\dagger}\ , \tag{2.73}$$

where $C_{jl\,1/2}^{m;m-\sigma}=\langle jl\tfrac{1}{2};m\mid l,m-\sigma;s=\tfrac{1}{2},\sigma\rangle$ is the Clebsch-Gordon coefficient projecting into the local f state. Typically, $l=3$ and $j=3\pm\frac{1}{2}$ in mixed-valence ions. In terms of these operators the mixing at each site is written

$$\mathscr{H}_{\rm mix}(\mathbf{R}_i)=\sum_{k,m}\frac{V(k)}{\sqrt{N}}[c_{km}^{\dagger}(\mathbf{R}_i)f_m(\mathbf{R}_i)b^{\dagger}(\mathbf{R}_i)+\text{H.c.}]\ . \tag{2.74}$$

In the case of the one-impurity model, the full Hamiltonian can be written down in terms of the local operators $c_{km}(\mathbf{R}=\mathbf{0})$ avoiding the need to ever explicitly consider the projection (2.73). In a real lattice we need to incorporate the details of the angular momentum structure.

To develop the formalism with maximum clarity, we shall forego a realistic angular momentum structure until the final section where this issue is addressed more fully. Instead we shall suppose that both the f electrons and the band electrons have a spin degeneracy of $N=2j+1$. In this case, the mixing at each site can be written

$$\mathscr{H}_{\rm mix}(\mathbf{R}_i)=\sum_{\mathbf{k},m}\frac{V(k)}{\sqrt{N}}[c_{\mathbf{k}m}^{\dagger}f_m(\mathbf{R}_i)b^{\dagger}(\mathbf{R}_i)e^{-i\mathbf{k}\cdot\mathbf{R}}+f_m^{\dagger}(\mathbf{R}_i)c_{\mathbf{k}m}b(\mathbf{R}_i)e^{i\mathbf{k}\cdot\mathbf{R}}]\ , \tag{2.75}$$

enabling us to write down the many-site version of the generalized Anderson model

$$\hat{\mathscr{H}}=\sum_{\mathbf{k},m}E(k)c_{\mathbf{k}m}^{\dagger}c_{\mathbf{k}m}+\sum_{\mathbf{R}_i m}E_f f_m^{\dagger}(\mathbf{R}_i)f_m(\mathbf{R}_i)+\sum_{\mathbf{R}_i}\mathscr{H}_{\rm mix}(\mathbf{R}_i)+\sum_{\mathbf{R}_i}\lambda(\mathbf{R}_i)\hat{Q}(\mathbf{R}_i)\ , \tag{2.76}$$

where

$$Q(\mathbf{R}_i)=\sum_{m,\mathbf{R}_i}f_m^{\dagger}(\mathbf{R}_i)f_m(\mathbf{R}_i)+b^{\dagger}(\mathbf{R}_i)b(\mathbf{R}_i) \tag{2.77}$$

and we associate a chemical potential $\lambda(\mathbf{R}_i)$ with each conserved charge $Q(\mathbf{R}_i)$. In the limit $E_f\ll 0$, this model reverts to a lattice version of the Coqblin-Schrieffer model with a spin interaction $-(J/N)\hat{\sigma}^{\dagger}(\mathbf{R}_i)\hat{\sigma}(\mathbf{R}_i)$ at each site, where

$$\hat{\sigma}(\mathbf{R}_i)=\sum_{\mathbf{k},m}f_m^{\dagger}(\mathbf{R}_i)c_{\mathbf{k}m}e^{i\mathbf{k}\cdot\mathbf{R}_i}\ .$$

The mean-field theory and the path-integral formalism develop along parallel lines to the one-impurity model. The partition function is written as a constrained functional integral

$$Z_{\rm MV}=\int_0^{2\pi i/\beta}\prod_{\mathbf{R}_j}\left[\frac{\beta d\lambda(R_j)}{2\pi i}\right]Z(\lambda_j)\exp\beta\left[\sum_j\lambda_j Q_j^0\right]\ , \tag{2.78}$$

where MV denotes mixed valence, and as before

$$Z(\lambda_j)=\text{Tr}e^{-\beta\hat{\mathscr{H}}[\lambda_j]}=\int\mathscr{D}[\bar{\psi},\psi]\mathscr{D}[\bar{b},b]e^{-\beta F[\bar{\psi},\psi,\bar{b},b]} \tag{2.79}$$

with

$$\beta F[\bar{\psi},\psi;\bar{b},b]=\int_0^{\beta}d\tau\left[\sum_i\left[\bar{\psi}_i(\tau)\frac{\partial}{\partial\tau}\psi_i(\tau)+\bar{b}_i\frac{\partial}{\partial\tau}b_i\right]+\mathscr{H}[\lambda_i]\right]\ . \tag{2.80}$$

The differences to the single-impurity case lie in the extended Hamiltonian, and the extended measures, which integrate over the λ_i, and the f electron and Bose fields for each site.

As before, the saddle points of the path integral are determined by the stationary point of the Bose-field effective action

$$\beta\Omega_{\rm eff}[\bar{b}_i,b_i,\lambda_i]=\int_0^\beta d\tau\sum_{k,i}\bar{b}(\mathbf{R}_i,\tau)\left[\frac{\partial}{\partial\tau}+\lambda_i\right]b(R_i,\tau)-\sum_i\beta\lambda_iQ_0+\beta F_\psi[\bar{b}_i,b_i] \tag{2.81}$$

from which we gain

$$\begin{aligned}\frac{\beta\delta\Omega_{\rm eff}}{\delta\bar{b}(\mathbf{R}_i,\tau)}&=\left[\frac{\partial}{\partial\tau}+\lambda(\mathbf{R}_i)\right]b(\tau)+\frac{1}{\sqrt{N}}\sum_{\mathbf{k},m}V(k)e^{-i\mathbf{k}R}\langle c^\dagger_{\mathbf{k}m}(\tau)f_m(\tau)\rangle=0\ ,\\ \frac{\beta\delta\Omega_{\rm eff}}{\delta\lambda(\mathbf{R}_i)}&=|b(\mathbf{R}_i,\tau)|^2+\langle\hat{n}_f(\mathbf{R}_i,\tau)\rangle-Q_0=0\ .\end{aligned} \tag{2.82}$$

The expectation values are determined from the motion of the electrons in the (c-number) dynamic Bose field

$$\mathscr{H}^*=\hat{\mathscr{H}}_{\rm band}+\sum_{\mathbf{R}_i}[E_f+\lambda(\mathbf{R}_i)]\hat{n}_f(\mathbf{R}_i)+\sum_{\mathbf{R}_i}\mathscr{H}^*_{\rm mix}(\mathbf{R}_i,\tau)\ , \tag{2.83}$$

where

$$\hat{\mathscr{H}}^*_{\rm mix}(R_j,\tau)=\sum_{\mathbf{R}_i}V(k)[\tilde{b}(\mathbf{R}_i,\tau)c^\dagger_{\mathbf{k}m}f_m(\mathbf{R}_i)\times e^{-i\mathbf{k}\cdot\mathbf{R}_i}+\text{H.c.}] \tag{2.84}$$

and

$$\tilde{b}(\mathbf{R}_i,\tau)=\frac{1}{\sqrt{N}}b(\mathbf{R}_i,\tau)\ . \tag{2.85}$$

The static thermodynamics demand $\tilde{b}(\mathbf{R}_i,\tau)=$const, leading to the simple mean-field equations

$$\begin{aligned}0&=\lambda(\mathbf{R}_i)\tilde{b}(\mathbf{R}_i)+\frac{1}{N}\sum_{\mathbf{k},m}V(k)\langle c^\dagger_{\mathbf{k}m}f_m(\mathbf{R}_i)\rangle e^{-i\mathbf{k}\cdot\mathbf{R}_i}\ ,\\ |\tilde{b}(\mathbf{R}_i)|^2&+\tilde{n}_f(\mathbf{R}_i)=q_0\ .\end{aligned} \tag{2.86}$$

To illustrate the application of these mean-field equations we shall consider (i) the case of two impurities and (ii) a simple lattice model. Related studies of the two-impurity model have been made by Lavagna for the Kondo model, using a different functional integral approach, and by Rasul for the infinite-U Anderson model using Brillouin-Wigner theory.[30,31] We shall contrast the results obtained here.

1. *Two impurities: mean-field behavior*

Suppose we have two impurities at $\pm\mathbf{R}/2$. Since the system is invariant under the parity operation $P:\mathbf{R}\to-\mathbf{R}$, the ground state will preserve this symmetry, so the mean-field calculation is simplified in advance by placing $\lambda(\mathbf{R}_1)=\lambda(\mathbf{R}_2)$ and $|\tilde{b}(\mathbf{R}_1)|=|\tilde{b}(\mathbf{R}_2)|$. Now $Q(\mathbf{R}_1)$ and $Q(\mathbf{R}_2)$ are independently conserved, so the phases of the Bose fields at each site can be independently modified without changing the energy, so we can choose $\tilde{b}(\mathbf{R}_1)=\tilde{b}(\mathbf{R}_2)=\mathbf{r}_0$. The mean-field Hamiltonian then becomes

$$\mathscr{H}^*=\mathscr{H}_{\rm band}+\tilde{E}_f(\hat{n}_{f1}+\tilde{n}_{f2})+\sum_{\mathbf{k},m}\tilde{V}(k)[c^\dagger_{\mathbf{k}m}(f_{1m}e^{i\mathbf{k}\cdot\mathbf{R}/2}+f_{2m}e^{-\mathbf{k}\cdot\mathbf{R}/2})+\text{H.c.}]\ , \tag{2.87}$$

where $\tilde{E}_f=E_f+\lambda$ and $\tilde{V}(k)=V(k)\tilde{r}_0$. The Hamiltonian can be split into two parts containing symmetric and antisymmetric eigenstates of the parity operator. We shall define symmetric ($P=+$) and antisymmetric ($P=-$) fermion states as follows:

$$\begin{aligned}f^P_m&=\frac{1}{\sqrt{2}}(f_{m1}+Pf_{m2})\ ,\\ c^{(+)}_{km}&=\frac{1}{[\mathscr{N}_+(k)]^{1/2}}\int\frac{d\Omega_k}{4\pi}\cos\left[\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right]c_{\mathbf{k}_m}\ ,\\ c^{(-)}_{km}&=\frac{i}{[\mathscr{N}_-(k)]^{1/2}}\int\frac{d\Omega_k}{4\pi}\sin\left[\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right]c_{\mathbf{k}m}\ ,\end{aligned} \tag{2.88}$$

where $\mathscr{N}_P(k)=\frac{1}{2}[1+Pj_0(k_FR)]$ and $j_0(x)=\sin x/x$. The antisymmetric and symmetric states are orthogonal

$$\begin{aligned}\{f^P_m,f^{\dagger P'}_{m'}\}&=\delta_{pp'}\delta_{mm'}\ ,\\ \{c^P_{km},c^{P'\dagger}_{k'm'}\}&=\delta_{pp'}\delta_{mm'}\delta_{kk'}\ ,\end{aligned} \tag{2.89}$$

and this enables us to write $\mathscr{H}^*=\sum_{P=\pm1}\mathscr{H}^P$, where

$$\mathscr{H}^P=\sum_{k,m}E(k)c^{P\dagger}_{km}c^P_{km}+\tilde{E}_fn^P_f+\sum_{k,m}\tilde{V}^P(k)(c^{P\dagger}_{km}f^P_m+\text{H.c.})\ . \tag{2.90}$$

Here, $\tilde{V}^P(k)=V^P(k)\tilde{r}_0$, $V^P(k)=V(k)[2\mathscr{N}_P(k)]^{1/2}$, and $\tilde{E}_f=E_f+\lambda$. The states of opposite parity are not mixed by the static mean-field potential, enabling us to treat these two channels as separate resonant scattering channels. Each channel can be treated at the mean-field level in an analogous manner to the one-impurity problem, so that the fermionic part of the free energy is

$$F^{\rm MF}_\psi=-Nk_BT\sum_{P=\pm1}\sum_{i\omega_n}\ln[\tilde{E}_f+\tilde{\Sigma}^{(P)}_f(i\omega_n)-i\omega_n]\ , \tag{2.91}$$

where

$$\Sigma^{(P)}_f(i\omega_n)=\tilde{r}_0^2\sum_{i\omega_n}\frac{V(k)^2}{i\omega_n-E(k)}[1+Pj_0(kR)]\ . \tag{2.92}$$

By analytically continuing the Matsubara sums, the fermionic part of the free energy can be written as the sum of two phase shifts

$$F_\psi=-N\int\frac{d\omega}{\pi}f(\omega)[\delta^{(+)}(\omega)+\delta^{(-)}(\omega)]\ , \tag{2.93}$$

where

$$\tan\delta^{(P)}(\omega)=\mathrm{Im}\{\ln|\tilde{E}_f+\Sigma_f^{(P)}(\omega-i\delta)-\omega]\}\ . \quad (2.94)$$

Provided that kR does not change significantly over the energy width of the resonance, then we can approximate $\Sigma_f^{(P)}(\omega-i\delta)$ by its value at the Fermi energy $\Sigma_f^{(P)}(\mu-i\delta)$. This condition is met provided that

$$R\frac{\partial k}{\partial E(k)}\bigg|_{k=k_F}\tilde{\Delta}=\left[\frac{R}{v_F}\right]\left[\frac{\tilde{\Delta}}{\hbar}\right]\ll 1\ . \quad (2.95)$$

This defines a "near field" around the local moments, within which $\Sigma_f^{(P)}(\omega)$ can be approximated. Now $R/v_F(\tilde{\Delta}/\hbar)=t/\tau_s$ where $t=R/v_F$ is the time for information to be transmitted between the two sites, and $\tau_s=\hbar/\tilde{\Delta}$ is the typical time scale for spin fluctuations of the local moment, so the near field is a region where conduction electrons travel between the impurities in a time which is short compared with the spin fluctuation time. This condition should be well satisfied in a typical mixed-valence or heavy-fermion system, as discussed by Rasul.[31] In a lattice $v_F\sim\varepsilon_F a$, where a is the lattice spacing and ε_F is the Fermi energy, so we can rewrite this expression as $R/a\ll\varepsilon_F/\tilde{\Delta}$. In a real system, $\varepsilon_F/\tilde{\Delta}\sim 100-1000$, so the "near field" of a mixed-valence ion is a vast region of $\sim 10^2-10^3$ lattice spacings about the ion.

In the case of the one-impurity problem, the real part of $\Sigma_f(\mu)$ can be set to zero by choosing a symmetric conduction band, and any departures from the symmetric case can be accommodated by a redefinition of E_f^* or the Kondo coupling constant. For two impurities, however, this is not true, since $\mathrm{Re}\Sigma_f^{(+)}\neq\mathrm{Re}\Sigma_f^{(-)}$, and only the parity-independent real part of $\mathrm{Re}\Sigma_f^{(P)}$ can be made to vanish by forming a symmetric band. [Although it is worth noting that had we chosen a one-dimensional conduction band with linear dispersion, then the real part of $\Sigma_f(\mu)$ would actually have vanished.] The essential approximation for $\Sigma_f^{(P)}(\omega)$ will therefore be

$$\Sigma_f^{(P)}(\omega-i\delta)=P\tilde{t}+i\tilde{\Delta}[1+Pj_0(k_F R)]\ , \quad (2.96)$$

where the parameter t is the parity-dependent real part of $\Sigma_f^{(P)}(\mu)$, given by

$$\tilde{t}=\tilde{r}_0^2 t=\tilde{r}_0^2\sum_k\frac{V(k)^2}{\mu-E(k)}j_0(kR)\ . \quad (2.97)$$

The even and odd phase shifts are then given by

$$\tan[\delta^{(P)}(\omega)]=\frac{\tilde{\Delta}^{(P)}}{\tilde{E}_f^{(P)}-\omega} \quad (2.98)$$

with $E_f^{(P)}=\tilde{E}_f+P\tilde{t}$ and $\tilde{\Delta}^{(P)}=\tilde{\Delta}[1+Pj_0(k_F R)]$. The widths *and* positions of these two resonances are different.

The splitting of the f resonances can be thought of as the development of dispersion in the f electrons. The term $\tilde{t}$ could equally well have been generated by an intersite hopping term in the original generalized Anderson Hamiltonian.

$$\mathscr{H}_{\mathrm{hop}}=\frac{t_{\mathrm{hop}}}{N}(b_L^\dagger f_{1m}f_{2m}^\dagger b_2+\mathrm{H.c.})\ , \quad (2.99)$$

and interestingly enough, it would also arise if a Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction of the form

$$\mathscr{H}_{\mathrm{RKKY}}=\frac{K}{N}\sum_{m,m'}(f_{1m}^\dagger f_{2m}f_{2m'}^\dagger f_{1m'}) \quad (2.100)$$

has been included, which might be appropriate in the Coqblin-Schrieffer case. Such terms are generated by the leading $O(1/N)$ fluctuations about mean-field theory, so that even if they were not included originally, they would generally appear in a renormalization process.

The total splitting of the resonances is then given by

$$\tilde{t}_{\mathrm{eff}}=\tilde{r}_0^2(t+t_{\mathrm{hop}})+\frac{K}{N}\sum_m\langle f_{1m}^\dagger f_{2m}\rangle\ . \quad (2.101)$$

With the Lorentzian phase shifts, in analogous fashion to the one-impurity case, we can integrate the free energy to arrive at

$$\Omega^{\mathrm{MF}}=N\left[2\lambda\tilde{r}^2+\sum_{P=\pm1}\mathrm{Im}\left[2ik_BT\ln[\tilde{\Gamma}(\xi^{(P)})]-\xi^{(P)}\frac{\ln(D\beta)}{2\pi i}\right]\right]\ , \quad (2.102)$$

where $\xi^{(P)}=\tilde{E}_f^{(P)}+i\tilde{\Delta}^{(P)}$. The mean-field equations can then be obtained directly by differentiating Ω^{MF} with respect to $\tilde{r}$ and λ, which leads to

$$\tilde{E}_f+\tfrac{1}{2}\sum_{P=\pm1}\mathrm{Re}\left[\frac{\Delta^{(P)}-iPt}{\pi}\left[\tilde{\psi}(\xi^P)-\ln\frac{\Delta\beta}{2\pi^2 i}\right]\right]=E_f^*\ , \quad (2.103)$$

$$r_0^2+\tfrac{1}{2}\sum_{P=\pm1}\mathrm{Im}\left[\frac{1}{\pi}\left[\tilde{\psi}(\xi^P)-\ln\frac{\Delta\beta}{2\pi^2 i}\right]\right]=q_0\ ,$$

where $\Delta^{(P)}=\Delta[1+Pj_0(k_F R)]$.

For the case of a parabolic band, where $E(k)=\hbar^2k^2/2m$, choosing $V(k)=V$, a constant,

$$t=\frac{2\Delta}{\pi}\int_0^{k_D}\frac{dkk^2}{k_F^3}\frac{1}{1-(k/k_F)^2}j_0(kR)$$
$$=-\Delta\left[\frac{\cos(k_F R)}{k_F R}+\frac{1}{\pi k_F R}g(k_f R,k_D/k_F)\right]\ , \quad (2.104)$$

where $E(k_D)=D$ defines the upper cutoff. The function $g(x,y)$ is given by

$$g(x,y)=\mathrm{Im}\{e^{ix}\mathrm{Ei}[i(y-1)x]+e^{-ix}\mathrm{Ei}[i(y+1)x]\}\ , \quad (2.105)$$

where $\mathrm{Ei}(ix)=-\int_x^\infty ds\,(e^{is}/s)$ is the exponential integral function.

The choice of k_D/k_F sets the degree of conduction-band asymmetry and this in turn determines the amount of f-electron dispersion in the quasiparticle excitation spectrum. t only vanishes for particular values of R; however, for the special case that $k_D/k_F=1.196\ldots$, t vanishes at $R=0$ and $R=\infty$.

Finally, we note that as in the one-impurity model, we can take the Kondo limit, whereupon the digamma functions dominate the left-hand sides of (2.103), leading to the result

$$\frac{1}{2}\sum_{P=\pm 1}\mathrm{Re}\left\{\frac{1+P[j_0(k_FR)-i\gamma(R)]}{\pi}\left[\tilde{\psi}(\xi^P)-\ln\left[\frac{T_K\beta}{2\pi i}\right]\right]\right\}=0\ ,$$
$$\frac{1}{2}\sum_{P=\pm 1}\mathrm{Im}\left\{\frac{1}{\pi}\left[\tilde{\psi}(\xi^P)-\ln\left[\frac{T_K\beta}{2\pi i}\right]\right]\right\}=q_0\ , \tag{2.106}$$

where $\gamma(R)=t/\Delta=\tilde{t}/\tilde{\Delta}=(\rho)^{-1}\sum_k j_0(kR)/[\mu-E(k)]$.

We summarize this section as follows.

(a) We have found a coherent mean-field solution characterized by a Fermi liquid involving two nondegenerate Kondo resonances with different widths $\tilde{\Delta}^{\pm}=\tilde{\Delta}[1\pm\sin(k_FR)/(k_FR)]$ and different positions $\tilde{E}_f^{(P)}=\tilde{E}_f+P\tilde{t}$. Within this Fermi liquid, intersite propagation is related to the *difference* between the antisymmetric and symmetric propagators $G_f^{12}(\omega)=\frac{1}{2}[G_f^+(\omega)-G_f^-(\omega)]$. Unlike the Brillouin-Wigner treatment, multiple intrasite *and* intersite hopping of conduction electrons is included at the mean-field level.

(b) Although there are two relevant energy scales characterizing the two-impurity model $\tilde{\Delta}^{\pm}$, the crossover to strong coupling is independent of intersite interactions in the mean-field limit, for when $r_0^2\to 0$, Eqs. (2.103) revert to the single-impurity expression. Coherence develops once the symmetric Bose fluctuations become unstable and acquire a finite amplitude. In Sec. IV we will find that below this temperature, once the finite expectation value of the symmetric Bose field is included, there is no subsequent instability of the antisymmetric fluctuations, as suggested by Lavagna.[30]

(c) The amount of f dispersion in the quasiparticle Hamiltonian is dependent on the degree of conduction-band asymmetry. This is a new feature of the many-site problem that is preserved by the $1/N$ corrections.

In Sec. IV we will return to the two-impurity model to calculate its Fermi-liquid parameters and intersite correlations.

2. *Simplified lattice model*

The extension of the spin j model to the lattice is straightforward. If we normalize the Hamiltonian to the unit cell, the mixing term for the lattice has the form

$$\mathscr{H}_{\mathrm{mix}}=\frac{1}{(n_s)^{1/2}}\sum_{\mathbf{R},\mathbf{k},m}\frac{V(k)}{\sqrt{N}}[c^\dagger_{\mathbf{k}m}f_m(\mathbf{R})b^\dagger(\mathbf{R})e^{-i\mathbf{k}\cdot\mathbf{R}}+\mathrm{H.c.}]\ , \tag{2.107}$$

where n_s is the number of sites in the lattice. In the mean-field-limit translation symmetry implies that the static values of $\lambda(R)$ and $|\tilde{b}(R)|=\tilde{r}_0$ are constant at every site. Defining Bloch states for the f electrons, the renormalized Hamiltonian governing the mean-field behavior is

$$\hat{\mathscr{H}}=\sum_{\mathbf{k},\mathbf{G},m}E(\mathbf{k}+\mathbf{G})c^\dagger_{\mathbf{k}+\mathbf{G},m}c_{\mathbf{k}+\mathbf{G},m}+\sum_{\mathbf{k},m}\tilde{E}_{f_m}\dagger(\mathbf{k})f_m(\mathbf{k})+\sum_{\mathbf{k},\mathbf{G}}\tilde{V}(\mathbf{k}+\mathbf{G})(c^\dagger_{\mathbf{k}+\mathbf{G},m}f_{\mathbf{k}m}+\mathrm{H.c.})\ , \tag{2.108}$$

where $f^\dagger_{km}=1/(n_s)^{1/2}\sum_j f^\dagger_m(\mathbf{R})e^{i\mathbf{k}\cdot\mathbf{R}_j}$ and the sum over $\mathbf{k}$ is restricted to the first Brillouin zone. The vectors $\mathbf{G}$ are the reciprocal-lattice vectors. As before, $\tilde{E}_f=E_f+\lambda$ and $\tilde{V}(k)=V(k)\tilde{r}_0$. In terms of Bloch states, the mean field is defined by

$$\lambda\tilde{r}_0+\frac{1}{N}\sum_{\mathbf{k},\mathbf{G},m}V(\mathbf{k}+\mathbf{G})\langle c^\dagger_{\mathbf{k}+\mathbf{G},m}f_m(\mathbf{k})\rangle=0\ ,$$
$$\tilde{r}_0^2+\frac{1}{N}\sum_{\mathbf{k},m}\langle f^\dagger_m(\mathbf{k})f_m(\mathbf{k})\rangle=q_0\ . \tag{2.109}$$

We can calculate the expectation values from the Green's functions

$$G_f(\mathbf{k},\tau)=\langle Tf_m(\mathbf{k},\tau)f^\dagger_m(\mathbf{k},0)\rangle\ ,$$
$$D(\mathbf{k},\tau)=\sum_{\mathbf{G}}V(\mathbf{k}+\mathbf{G})\langle Tf_m(\mathbf{k},\tau)c^\dagger_{\mathbf{k}+\mathbf{G},m}(0)\rangle\ , \tag{2.110}$$

where, in Fourier components

$$G_f(\mathbf{k},i\omega_n)=[i\omega_n-\tilde{E}_f-\Sigma(\mathbf{k},i\omega_n)]^{-1}\ ,$$
$$D(\mathbf{k},i\omega_n)=\Sigma(\mathbf{k},i\omega_n)G_f(\mathbf{k},i\omega_n)\ , \tag{2.111}$$

and

$$\Sigma(\mathbf{k},i\omega_n)=\tilde{r}_0^2\sum_G|V(\mathbf{k}+\mathbf{G})|^2/[i\omega_n-E(\mathbf{k}+\mathbf{G})]\ . \tag{2.112}$$

The poles of $G_f(\mathbf{k},z)$ define a renormalized band with two branches on either side of the renormalized f-level $\tilde{E}_f$ given by

$$\varepsilon(\mathbf{k})=\tilde{E}_f+\Sigma(\mathbf{k},\varepsilon(\mathbf{k}))\ . \tag{2.113}$$

We shall assume for definiteness, that $\tilde{E}_f=E(k)$ for some $\mathbf{k}$ in the first zone. $\Sigma(\mathbf{k},\omega)$ is now conveniently separated into two terms $\Sigma(\mathbf{k},\omega)=\Sigma_0(\mathbf{k},\omega)+\tilde{r}_0^2t(\mathbf{k},\omega)$, where

$$\Sigma_0(\mathbf{k},\omega)=\frac{\tilde{V}(\mathbf{k})^2}{\omega-E(k)} \tag{2.114}$$

is a singular function for $\omega\sim\varepsilon(\mathbf{k})$ and

$$t(\mathbf{k},\omega)=\sum_{\mathbf{G}(\neq 0)}\frac{V(\mathbf{k}+\mathbf{G})^2}{\omega-E(\mathbf{k}+\mathbf{G})} \tag{2.115}$$

is a smoothly varying function for $\omega\sim\varepsilon(\mathbf{k})$. In general, since $\tilde{V}(k)$ and $\tilde{E}_f$ are much smaller than the width of the conduction bands, we can approximate $t(\mathbf{k},\omega)\approx t(\mathbf{k},\mu)$, where μ is the chemical potential. The eigenvalue equation now becomes

$$\varepsilon(\mathbf{k})=\tilde{E}_f+\tilde{r}_0^2t(\mathbf{k},\mu)+\Sigma_0(\mathbf{k},\varepsilon(\mathbf{k}))\ . \tag{2.116}$$

Without the final term, this would give rise to an f band

with weak dispersion given by $\tilde{E}_f(\mathbf{k})=\tilde{E}_f+\tilde{r}_0^2 t(\mathbf{k},\mu)$. This is a consequence of admixture with the higher conduction bands. The final term introduces the hybridization with the conduction band in the first zone, and leads to two poles in $G_f(\mathbf{k},\omega)$, given by $\omega=\varepsilon_k^\alpha$ ($\alpha=\pm1$), where

$$\varepsilon^{\pm}(\mathbf{k})=\tfrac{1}{2}(\tilde{E}_f(\mathbf{k})+E(k) \pm\{[\tilde{E}_f(\mathbf{k})-E(k)]^2+4\tilde{r}_0^2 V(\mathbf{k})^2\}^{1/2}) . \quad (2.117)$$

Note, that the mixing with the higher bands will sometimes lead to sufficient dispersion in $\tilde{E}_f(\mathbf{k})$ to eradicate the "hybridization gap" between the lower and upper band.

The mixing Green's function determines the degree of mixing between band and f electrons

$$\frac{1}{N}\sum_{k,\mathbf{k},m}\tilde{V}(k)\langle c^\dagger_{\mathbf{k}+\mathbf{K},m} f_m(\mathbf{k})\rangle=\beta^{-1}\sum_{\mathbf{k},i\omega_n} D(\mathbf{k},i\omega_n) \quad (2.118)$$

and by contour integrations, distorting the contours around the poles $\varepsilon^\alpha(\mathbf{k})$, we can determine λ, yielding

$$\tilde{E}_f=E_f+\sum_{\mathbf{G}}\int\frac{d^3k}{(2\pi)^3}|V(\mathbf{k}+\mathbf{G})|^2 \times\left[\frac{f(\varepsilon^-(\mathbf{k}))-f(\varepsilon^+(\mathbf{k}+\mathbf{G}))}{\varepsilon^+(\mathbf{k}+\mathbf{G})-\varepsilon^-(\mathbf{k})}\right], \quad (2.119)$$

where the integrations are over the first Brillouin zone. As in the one-impurity case, the renormalization of the f level involves excitations extending to the upper band edge, leading to a dependence of $\tilde{E}_f$ on the bandwidth. We can extract this dependence by defining an invariant f level

$$E_f^*=E_f+\sum_{\mathbf{G}}\int\frac{d^3k}{(2\pi)^2}|V(\mathbf{k}+\mathbf{G})|^2 \frac{\Theta(-E(\mathbf{k}+\mathbf{G}))}{\Delta/\pi-E(\mathbf{k}+\mathbf{G})} , \quad (2.120)$$

where $\Delta=\pi\rho(\varepsilon_F)|V(k_F)|^2$ as before. For an artificial Lorentzian density of states with no k dependence of the hybridization, $\Delta(\varepsilon)=\Delta D^2/(\varepsilon^2+D^2)$, as assumed in the single-impurity model, $E_f^*=E_f+(\Delta/\pi)\ln(D\pi/\Delta)$. In general, the detailed cutoff dependence will of course be more complicated. E_f^* contains the information about the local high-frequency charge fluctuations which contribute the major renormalization of E_f. In terms of E_f^*

$$\tilde{E}_f=E_f^*+\sum_{\mathbf{G}}\int\frac{d^3k}{(2\pi)^2}|V(\mathbf{k}+\mathbf{G})|^2\left[\frac{f(\varepsilon^-(\mathbf{k}))-f(\varepsilon^+(\mathbf{k}+\mathbf{G}))}{\varepsilon^+(\mathbf{k}+\mathbf{G})-\varepsilon^-(\mathbf{k})}-\frac{\Theta(-E(\mathbf{k}+\mathbf{G}))}{\Delta/\pi-E(\mathbf{k}+\mathbf{G})}\right] \quad (2.121)$$

and the integral does not depend on details of the high-energy cutoff. The dominant contribution to the remainder is derived from excitations near the Fermi energy, enabling us to approximate $V(k)$ and the density of states by their value at the Fermi energy. We can evaluate this integral precisely, provided that the k dependence of $V(k)$ and the f-band dispersion $t(\mathbf{k},\mu)$ are ignored. By making these approximations and changing variables to $\varepsilon=\varepsilon^{\pm}(\mathbf{k})$ in the first term of the integrand and $\varepsilon=E(k)$ in the last term then yields

$$\tilde{E}_f=E_f^*+\frac{\Delta}{\pi}\int_{-\infty}^{+\infty}d\varepsilon\left[\frac{f(\varepsilon)}{\tilde{E}_f-\varepsilon}-\frac{\Theta(-\varepsilon)}{\Delta/\pi-\varepsilon}\right] =E_f^*-\frac{\Delta}{\pi}\left[\mathrm{Re}\tilde{\psi}(\tilde{E}_f)-\ln\frac{\Delta\beta}{2\pi^2}\right], \quad (2.122)$$

which is very similar to the single-impurity result reducing to

$$\tilde{E}_f+\frac{\Delta}{\pi}\ln\frac{\tilde{E}_f\pi}{\Delta}=E_f^* \quad (2.123)$$

at $T=0$.

The f occupation $\tilde{n}_f=\langle\hat{n}_f\rangle/N$ can be calculated from the f propagator

$$\tilde{n}_f=\beta^{-1}\sum_{\mathbf{k},i\omega_n}G_f(\mathbf{k},i\omega_n) . \quad (2.124)$$

We shall expand $G_f(\mathbf{k},i\omega_n)$ as

$$G_f(\mathbf{k},i\omega_n)=G^+(\mathbf{k},i\omega_n)+G^-(\mathbf{k},i\omega_n)-G_b(\mathbf{k},i\omega_n) , \quad (2.125)$$

where $G^{\pm}(\mathbf{k},i\omega_n)=[i\omega_n-\varepsilon^{\pm}(\mathbf{k})]^{-1}$ and

$$G_b(\mathbf{k},i\omega_n)=\{i\omega_n-E(\mathbf{k})-|\tilde{V}(k)|^2/[i\omega_n-\tilde{E}_f(\mathbf{k})]\}^{-1} \quad (2.126)$$

is the band-electron propagator in the presence of the strong resonant scattering at each site. Carrying out (2.124) as a contour integral then yields

$$\tilde{n}_f=V_0\int\frac{d^3k}{(2\pi)^3}[f(\varepsilon_k^+)+f(\varepsilon_k^-)-f(E(k))]-\tilde{n}_p, \quad (2.127)$$

where

$$\tilde{n}_p=V_0\int\frac{d^3k}{(2\pi)^2}(\langle c^\dagger_{\mathbf{k}m}c_{\mathbf{k}m}\rangle|_{\tilde{r}\neq0}-\langle c^\dagger_{\mathbf{k}m}c_{\mathbf{k}m}\rangle|_{\tilde{r}=0}) \quad (2.128)$$

is the polarization of the band electrons by the renormalized scattering potential. By expanding $\tilde{n}_p$ to leading order in $|\tilde{V}(k)|^2$, we find $\tilde{n}_p=0(\Delta\tilde{r}_0^2/D)\ll1$, showing that the band electrons are essentially unpolarized by the mixed-valence lattice (this is Anderson's compensation theorem, generalized to the lattice). The main contribution to $\tilde{n}_f$ is recognized as the increase in the Fermi-surface volume due to the renormalized scattering potential.

The two results (2.122) and (2.127) illustrate an impor-

tant property of the lattice, that while the renormalized position of the f level and hence the bulk energetics of the lattice are determined by the local fluctuations, leading to a similarity between the mean-field expressions for $\tilde{E}_f$, the coherence effects of repeated scattering near the Fermi surface lead to quite different sum rules governing the f occupation. Equation (2.127) enables us to write the final mean-field constraint equation $\tilde{n}_f+\tilde{r}_0^2=q_0$ as

$$\tilde{r}_0^2+\delta V_{\rm FS}/(2\pi)^3=q_0 \ , \tag{2.129}$$

where $\delta V_{\rm FS}$ is the change in the Fermi-surface volume. Martin[32] has emphasized the importance of the Fermi-surface sum rules for the mixed-valence lattice, and it is satisfying to see this feature naturally incorporated at the mean-field level.

H. Relationship with earlier approaches

It is illuminating to examine the relationship between this formalism and earlier approaches. Following Anderson's suggestion of using $1/N$ as an expansion parameter in mixed valence,[33] Ramakrishnan[34] showed using a Brillouin-Wigner perturbation theory for the infinite-U Anderson model, that a perturbation expansion can be made in powers of $1/N$. Gunnarson and Schönhammer[7] subsequently showed that at zero temperature, this is equivalent to using the Varma-Yafet (VY) variational wave function[35]

$$|\psi_{\rm VY}\rangle=\left[1+\sum_{k,m}\alpha(k)f_m^\dagger c_{km}\right]|0\rangle \ , \tag{2.130}$$

where $|0\rangle$ is the unperturbed Fermi sea. The ground-state energy yielded from this variational wave function is

$$E_0=E_f-\tilde{E} \tag{2.131}$$

where

$$\tilde{E}+\frac{\Delta}{\pi}\ln\left[\frac{\tilde{E}\pi}{\Delta}\right]=E_f^* \ . \tag{2.132}$$

If we had derived our mean-field theory using a variational wave function, we would have used the coherent state

$$|\theta\rangle=\prod_m\left[1+\sum_k\alpha(k)e^{i\theta}f_m^\dagger c_{km}\right]\exp(re^{i\theta}\hat{b}^\dagger)|0\rangle \ . \tag{2.133}$$

The $Q=1$ projection of $|\theta\rangle$ is

$$\int\frac{d\theta}{2\pi}e^{-i\theta}|\theta\rangle=\left[r\hat{b}^\dagger+\sum_{k,m}\alpha(k)f_m^\dagger c_{km}\right]|0\rangle \ , \tag{2.134}$$

which has the same form as the VY wave function, once we have made the identification $\hat{b}^\dagger|0\rangle\equiv|f^0\rangle$ and $f_m^\dagger|0\rangle=|f^{1;jm}\rangle$. Now clearly $|\theta\rangle$ involves a range of different Q, such that the average $\langle\hat{Q}\rangle=qN$. Despite this distribution of Q, we find that the ground-state energy is given by

$$E_0=N\left[q(E_f-\tilde{E}_f)+\tilde{E}_f\left[\tilde{n}_f-\frac{1}{\pi}\tan(\pi\tilde{n}_f)\right]\right] \ , \tag{2.135}$$

where $\xi=\tilde{E}_f+i\Delta(q-\tilde{n}_f)$ satisfies $\xi+(\Delta/\pi)\ln(\xi\pi/\Delta)=E_f^*+i\Delta q$. Setting $\tilde{n}_f=n_f/N$, $q=1/N$, we find that our result reverts to the variational result $E_0=E_f-\tilde{E}_f$. This equivalence of the ground-state energy for the single-impurity model was first shown by Read and Newns.

For the case of the lattice, the mean-field treatment that we employ is equivalent to the following coherent state representation of the ground state

$$|\{\theta_j\}\rangle=\prod_{\mathbf{k},m}\left[\alpha(\mathbf{k})c_{\mathbf{k}m}^\dagger+\beta(\mathbf{k})\sum_j e^{i(\theta_j+\mathbf{k}\cdot\mathbf{R}_j)}f_m^{\dagger(j)}\right]\times\exp\left[r\sum_j e^{i\theta_j}\hat{b}^{\dagger(j)}\right]|0\rangle \ , \tag{2.136}$$

where $|0\rangle$ is the empty vacuum. The projection of this state onto a state of definite $Q=1$ is

$$|\psi(Q=1)\rangle=\int\prod_j\frac{d\theta_j}{2\pi}e^{-i\theta_j}|\{\theta_j\}\rangle \ , \tag{2.137}$$

which when expanded is identical to the variational state considered by Brandow.[36] The derivation of the leading order ground-state energy is much simpler in the coherent state representation. We note in passing, that a similar approach enables the Gutzwiller ground state to be simply rederived for the Hubbard model.[37]

III. $1/N$ FLUCTUATIONS

A. Relationship between zero modes and strong coupling

Our mean-field saddle-point equations furnish the starting point for a controlled $1/N$ expansion. In carrying out this $1/N$ expansion it is helpful to regard the large-N limit as a quasiclassical limit of the model, where $1/N$ plays the role of Planck's constant and the mean-field equations describe the classical trajectory. Fluctuations about this path can be viewed as quantum fluctuations, and exactly as in a conventional classical limit, the expansion about the classical trajectory is carried out by means of a loop expansion in $1/N$ ($\equiv\hbar$). In this large-N limit, the fermion bilinear operators

$$O_{ij}(t)=(1/N)\textstyle\sum_{m\in[-j,j]}[\psi_{im}^\dagger(t)\psi_{jm}(t)]$$

and the rescaled Bose field $\tilde{b}(t)=b(t)/\sqrt{N}$ behave as classical variables,[22,38] defining a classical field theory.

The Bose field in our model describes the collective electronic motions of the heavy Fermi liquid. At finite degeneracy, the Bose field is not rigid as in the mean-field limit, and it undergoes small fluctuations about the classical trajectory. These fluctuations contain much of the physics of the Fermi liquid. For instance, motions of the quasiparticles generate additional fluctuations which create interactions between quasiparticles. We will calculate the Fermi-liquid parameters by calculating the linear response of the Bose field to the quasiparticles.

We emphasize earlier how the zero-mode fluctuations of the Bose condensate are responsible for the divergence of the interactions in strong coupling. As in any theory with a continuous symmetry, care is required in treating

these fluctuations, and the calculation is simplified by respecting the underlying symmetry in one's coordinate system.

The problem of dealing with the zero modes has been elegantly solved by Read and Newns, who have shown how the infrared divergences associated with strong coupling in the Kondo problem are controlled by expressing the fluctuations in terms of the amplitude r and phase velocity $\partial\theta/\partial\tau=\dot{\theta}$ associated with the Bose field $b=re^{i\theta}$. Our ability to express the dynamics entirely in these Bose coordinates arises because of the Q conservation symmetry which ensures that static phase shifts in the Bose field do not affect the dynamics. (The Hamiltonian and Lagrangian are invariant under the symmetry operation $b\rightarrow be^{i\theta}$, $f\rightarrow fe^{i\theta}$.)

Read and Newns exploit this symmetry to carry out a simple gauge transformation on the fields, in which the phase associated with the Bose field is factored out of both the Bose and f-electron fields

$$\begin{aligned} b(\tau)&=r(\tau)e^{i\theta(\tau)}\ , \\ f_m(\tau)&=f'_m(\tau)e^{i\theta(\tau)}\ . \end{aligned} \tag{3.1}$$

By factoring out the phase fluctuations the divergences are removed and one obtains an equivalent description of the dynamics which is appropriate to the Fermi liquid. Whereas the untransformed fields have divergent strong-coupling interactions at low energies, the transformed Fermi fields have well behaved and finite interactions at low energies. Read and Newns interpret the redefined f-electron fields as the quasiparticles of the strongly coupled Fermi liquid, calling the new coordinate system the "quasiparticle gauge."

The relationship between the bare f electrons and the quasiparticles is illustrated by the full f propagator

$$\begin{aligned} \mathcal{G}_{fm}(\tau)&=\langle TX_{0m}(\tau)X_{m0}(0)\rangle \\ &=\langle Tb^{\dagger}(\tau)f_m(\tau)f_m^{\dagger}(0)b(0)\rangle\ , \end{aligned} \tag{3.2}$$

which is expressed as

$$\mathcal{G}_{fm}(\tau)=\langle Tr(\tau)f_m(\tau)f_m^{\dagger}(0)r(0)\rangle \tag{3.3}$$

in the transformed fields. A key feature to emerge in the calculation of the correlations is that at long times and low frequencies the dynamic correlations between the transformed Bose and Fermi fields become weak leading to well-defined quasiparticle excitations. In fact, at long times

$$\lim_{\tau\rightarrow\infty}\mathcal{G}_{fm}(\tau)=r_0^2\langle Tf_m(\tau)f_m^{\dagger}(0)\rangle\ , \tag{3.4}$$

where $r_0^2=\lim_{\tau\rightarrow\infty}\langle r(\tau)r(0)\rangle$ and $\langle f_m(\tau)f_m^{\dagger}(0)\rangle$ is essentially the f propagator of the mean-field limit with renormalizations to $\tilde{E}_f$ and $\tilde{\Delta}$ caused by high-frequency zero-point fluctuations. This enables us to interpret

$$r_0^2=Z_f \tag{3.5}$$

as the quasiparticle pole strength of the f electrons. At the mean-field level $r_0^2=Q-n_f$, which exemplifies why the wave-function renormalization factor becomes smallest in the Kondo regime, where n_f becomes close to Q, and there are very few "holes" present in the ground state into which conduction electrons can hop.

This switch to polar coordinates clarifies the almost-broken-symmetry character of the strong-coupling regime. Phase fluctuations ensure that in the original coordinate system

$$\langle b(\tau)b^{\dagger}(0)\rangle\sim\langle e^{i\theta(\tau)}e^{-i\theta(0)}\rangle\rightarrow 0 \tag{3.6}$$

as $\tau\rightarrow\infty$ so there is no true broken symmetry. However, in the polar coordinates

$$\lim_{\tau\rightarrow\infty}\langle r(\tau)r(0)\rangle=r_0^2 \tag{3.7}$$

and the almost broken symmetry is characterized by the development of low-frequency radial fluctuations in strong coupling. We will now proceed to demonstrate these features, illustrating the calculations using the one- and two-impurity models.

B. Strong-coupling dynamics

Extending our calculations entails expanding the effective free-energy functional

$$\beta\Omega_{\rm eff}[\bar{b},b,\lambda]=\int_0^{\beta}d\tau[\bar{b}(\tau)b(\tau)-Q_0]\lambda+\beta F_{\Psi}[\bar{b},b,\lambda] \tag{3.8}$$

in terms of small fluctuations $b(\tau)=b_0+\delta b(\tau)$ about the saddle point. In weak coupling, this is very straightforward, for the equilibrium value of the Bose field is zero. Strong coupling presents a problem because zero-mode fluctuations lead to unbounded phase fluctuations, so that $\langle\delta\theta^2\rangle$ is divergent. If one attempts to expand about the broken-symmetry state using the current description of the fields, these infrared divergences require special regulation, although of course, in physical quantities the divergences all cancel.[39]

Rather than following this path we shall employ Newns and Read's transformation to polar coordinates, which we now examine in detail. The factorization contained in this simple gauge transformation leads to new dynamics for the transformed fields. Two aspects of the transformation must be considered: (i) the changes in measure which must be introduced into the path integral and (ii) the modified Lagrangian.

The Jacobian associated with the transformation of the Fermi fields involves a product of phase factors and is therefore 1, leaving the fermion part of the measure unchanged. The new measure for the transformed Bose fields is now

$$\mathcal{D}[u,\theta]=\prod_{\tau}\frac{du(\tau)d\theta(\tau)}{2\pi}\ , \tag{3.9}$$

where $u(\tau)=r^2(\tau)$.

In deriving this measure we have to formally go through the process of transforming first to "momentum-space" coordinates (p,q) whose corresponding operators are defined by $\hat{p}+i\hat{q}=\hat{b}$, in terms of which we have a real measure for the path integral $\prod dpdq/\pi$. We then can define the functions $r(\tau)$ and $\theta(\tau)$ by

$p(\tau)+iq(\tau)=r(\tau)e^{i\theta(\tau)}$ to derive the new measure. We shall write of $b(\tau)=r(\tau)e^{i\theta(\tau)}$ as a *shorthand* for this sequence of transformations, bearing in mind that strictly $b(\tau)$ and $\bar{b}(\tau)$ are independent functions, not complex conjugates.[40]

The transformed Lagrangian contains a new interaction term $i\dot{\theta}(Q-Q_0)$ coming from the derivative terms in the free-energy functional:

$$\int \left[\bar{f}_m(\tau)\frac{\partial}{\partial(\tau)}f_m(\tau)+\bar{b}(\tau)\frac{\partial}{\partial(\tau)}b(\tau)\right]=\int_0^\beta d\tau\left[\bar{f}'_m(\tau)\frac{\partial}{\partial(\tau)}f'_m(\tau)+i\dot{\theta}(\tau)[Q(\tau)-Q_0]\right], \tag{3.10}$$

where $\dot{\theta}=\partial\theta(\tau)/\partial\tau$. The periodic boundary conditions in the Bose field ensure that we can remove the total derivative term $r(\tau)\partial r/\partial\tau(\tau)$ and add $-i\dot{\theta}(\tau)Q_0$ into the functional.

We now have to carefully consider the integration about the broken-symmetry state. When we integrate over θ we must be careful to allow for paths where θ changes by multiples of 2π, and the most general path has the form

$$\theta_m(\tau)=(k_BT)^{1/2}\sum_{n\neq 0}\theta_n e^{-i\nu_n\tau}+m(2\pi k_BT)\tau+\theta_0 . \tag{3.11}$$

When we integrate over θ, we will factor out the integration over the constant phase, writing

$$\prod_\tau \frac{d\dot{\theta}(\tau)}{2\pi}=\sum_{m=-\infty}^{\infty}\frac{d\dot{\theta}_0}{2\pi}\prod_\tau\frac{d\dot{\theta}(\tau)}{2\pi}\delta\left[\beta^{-1}\int_0^\beta d\tau\,\dot{\theta}(\tau)-2\pi m\right] . \tag{3.12}$$

Physical variables commute with $\hat{Q}$ and are therefore independent of θ_0, enabling us to remove the average over θ_0. In Fourier coordinates this becomes

$$\mathscr{D}[\theta]=\sum_m\prod_{n(\neq 0)}\left[\frac{k_BT}{2\pi}\right]d\theta_n , \tag{3.13}$$

where the sum is over the paths of different winding number m. As in (3.11) we can expand the angular velocity as

$$\dot{\theta}(\tau)=2\pi k_BTm+(k_BT)^{1/2}\sum_n\dot{\theta}_n e^{-i\nu_n\tau} , \tag{3.14}$$

where only integral multiples of $2\pi/\beta$ are allowed as the constant term. In terms of $\dot{\theta}$ the measure $\mathscr{D}[\theta]$ is

$$\mathscr{D}[\theta]=\sum_m\prod_{n(\neq 0)}\frac{(k_BT)^{1/2}}{2\pi i\nu_n}d\dot{\theta}_n . \tag{3.15}$$

We note that the integral over the chemical potential

$$\int_{\lambda_0}^{\lambda_0+2\pi ik_BT}\frac{d\lambda\beta}{2\pi i}\{\cdots\} , \tag{3.16}$$

where λ_0 is the static chemical potential determined by the saddle point, can be written

$$\int_0^{2\pi/\beta}\frac{d\Omega_0\beta}{2\pi}\{\cdots\} , \tag{3.17}$$

where $\lambda=i\Omega_0+\lambda_0$. But in the Lagrangian, Ω_0 and $\dot{\theta}$ enter in the same way

$$\{\lambda_0+i[\Omega_0+\dot{\theta}(\tau)]\}[Q(\tau)-Q_0] , \tag{3.18}$$

so if we define $\dot{\theta}'(\tau)=\dot{\theta}+\Omega_0$, then the new function

$$\dot{\theta}'(\tau)=(\Omega_0+2\pi k_BTm)+(k_BT)^{1/2}\sum_n\dot{\theta}_n e^{-i\nu_n\tau} \tag{3.19}$$

has a static value $\Omega_0+2\pi k_BTm$ that runs from $-\infty$ to ∞, allowing us to write

$$\mathscr{D}[\theta]=\mathscr{N}\prod_\tau\left[\frac{d\dot{\theta}'(\tau)\beta}{2\pi}\right]=\mathscr{D}[\dot{\theta}'] , \tag{3.20}$$

where $\mathscr{N}=\prod_{n\neq 0}(\beta i\nu_n)^{-1}$ is the normalization factor. Thus, by including paths with any winding number, we are able to incorporate the constraint naturally as part of the dynamics. We shall now suppress the prime on $\dot{\theta}'$ in subsequent expressions.

The partition function in the transformed fields is then written

$$Z_{\rm MV}=\int\mathscr{D}[r,\dot{\theta}]\mathscr{D}[\bar{\psi},\psi]\exp\left[-\int_0^\beta d\tau\mathscr{L}(\tau)\right] \tag{3.21}$$

where $\mathscr{L}(\tau)$ is the transformed Lagrangian, given by

$$\mathscr{L}(\tau)=\sum_i\bar{\psi}_i\frac{\partial}{\partial(\tau)}\psi_i+H'[\bar{\psi},\psi,r,\dot{\theta}]+\lambda_0[r^2(\tau)-Q_0] \tag{3.22}$$

and

$$\hat{H}'=\sum_{k,m}E(k)c^\dagger_{km}c_{km}+\sum_m\tilde{E}_f f^\dagger_m f_m+\hat{H}_{\rm int} \tag{3.23}$$

with

$$\hat{H}_{\rm int}=r(\tau)\sum_{k,m}\frac{V(k)}{\sqrt{N}}(c^\dagger_{km}f_m+f^\dagger_m c_{km})+i\dot{\theta}(\tau)(\hat{Q}-Q_0) , \tag{3.24}$$

where $f_m(\tau)$ refers to the gauge transformed f electron field and

$$\mathscr{D}[r,\dot{\theta}]=\prod_\tau dr^2(\tau)\prod\frac{d\dot{\theta}(\tau)}{2\pi} \tag{3.25}$$

defines the measure over the Bose fields.

In the transformed coordinates the Fermion part of the Lagrangian no longer contains the explicit Q conservation symmetry $b\to be^{i\theta}$, $f\to fe^{i\theta}$, and now the integral over $\dot{\theta}$ imposes Q conservation on the dynamics.

Our derivation is essentially that of Read and Newns, with two formal differences: it extends their result to arbitrary Q_0 enabling a true large-N limit to be found, and it carefully shows that it is unnecessary to promote the

chemical potential to a dynamical variable if one incorporates all paths with multiple winding number.

As in the Cartesian system, we can integrate over the Fermi fields for a fixed Bose-field configuration, defining a Bose effective free-energy functional

$$\beta\Omega_{\rm eff}[r,\dot\theta]=\int_0^\beta d\tau[r^2(\tau)-Q_0][\lambda_0+\dot\theta(\tau)]+\beta F_\psi\ , \tag{3.26}$$

where the Fermion part F_Ψ is given in shorthand notation as

$$\beta F_\psi=-\mathrm{Tr}\ln[(\hat G_f^{(0)})^{-1}+i\dot\theta(\tau)\hat n_f+r(\tau)\Sigma_f(\tau-\tau')r(\tau')]\ . \tag{3.27}$$

We can actually relate this result to the perturbative expression for F_Ψ (3.27) in the Cartesian gauge, which we shall expand as

$$\beta F_\Psi[\bar b,b]=-\mathrm{Tr}\ln[(G_f^{(0)})^{-1}]+\sum_{n=1}^{\infty}\frac{1}{n}\int_0^\beta\prod_{\substack{r=1\\ j=2r-1}}d\tau_{j+1}d\tau_j\Sigma_f(\tau_{j+2}-\tau_{j+1})\bar b(\tau_{j+1})G_f^{(0)}(\tau_{j+1}-\tau_j)b(\tau_j)\ , \tag{3.28}$$

where the subscripts on the τ are evaluated mod$(2n)$. In (3.28) each propagator $G_f^{(0)}(\tau)$ is sandwiched between Bose fields

$$\bar b(\tau')G_f^{(0)}(\tau'-\tau)b(\tau)\ . \tag{3.29}$$

To leading order in the fluctuations we can write

$$\begin{aligned}\bar b(\tau')G_f^{(0)}(\tau'-\tau)b(\tau)=&\,r(\tau')G_f^{(0)}(\tau'-\tau)r(\tau)\\&-ir_0^2G^{(0)}(\tau'-\tau)\\&\times[\delta\theta(\tau)-\delta\theta(0)]\ .\end{aligned} \tag{3.30}$$

The first term is merely the contraction of $G_f^{(0)}(\tau-\tau')$ with the radial interaction term, while expanding the second term in frequency space gives

$$\begin{aligned}&-iG_f^{(0)}(\tau'-\tau)[\delta\theta(\tau)-\delta\theta(\tau')]\\&\qquad=\frac{1}{\beta^2}\sum_{n,m}\Gamma(i\omega_m,i\nu_n)e^{-i[(\omega_m+\nu_n)\tau-\omega_m\tau']}\ ,\end{aligned} \tag{3.31}$$

where

$$\Gamma(i\omega_m,i\nu_n)=-i\nu_n\theta_nG_f^{(0)}(i\omega_n+i\omega_m)G^{(0)}(i\omega_m)\ . \tag{3.32}$$

This can be recognized as the contraction of the f propagator fields with the angular fluctuation fields. The power of the path integral is in confirming that the two expressions for F_Ψ, (3.27) and (3.28), are equivalent to all orders.

C. Gaussian approximation

For small fluctuations about our mean-field limit, the Bose measure can be approximated as locally Cartesian

$$\mathscr{D}[r,\dot\theta]=\mathscr{N}'\prod_\tau dr(\tau)d\dot\theta(\tau)\ , \tag{3.33}$$

where $\mathscr{N}'$ is the appropriate normalization constant. Going beyond the Gaussian fluctuations to calculate the $O(1/N^2)$ effects requires working with the full measure and restricting the radial fluctuations to being solely positive, a task which is beyond the work presented here. Nevertheless, inclusion of the small Gaussian fluctuations provides a theory which contains much of the important physics of strong coupling. This provides us with a "semiclassical" theory of mixed valence.

When we expand the Lagrangian about the saddle point we find

$$\mathscr{L}(\tau)=\bar\psi_i\frac{\partial}{\partial\tau}\psi_i+\mathscr{H}^*[\bar\psi,\psi]+N(\tilde r_0^2-q_0)+\mathscr{H}_{\rm int}\ , \tag{3.34}$$

where $\mathscr{H}^*[\bar\psi,\psi]$ is the mean-field Hamiltonian and

$$\begin{aligned}\mathscr{H}_{\rm int}=&\sum_{k,m}V(k)(f_m^\dagger c_{km}+c_{km}^\dagger f_m)\delta\tilde r(\tau)+i\dot\theta\hat n_f\\&+N[\lambda\delta\tilde r(\tau)^2+2i\tilde r_0\delta\tilde r(\tau)\dot\theta(\tau)]\ .\end{aligned} \tag{3.35}$$

All linear terms in the fields vanish by the saddle point condition.

We shall introduce the nomenclature

$$\bar{\mathbf{r}}(\tau)=(\delta\tilde r(\tau),i\tilde r_0\dot\theta(\tau))\ , \tag{3.36}$$

where $\sqrt{N}\,\delta\tilde r=r(\tau)-r_0(\tau)$ and $\sqrt{N}\,\tilde r_0=r_0$ are rescaled fields. Then to second order

$$\begin{aligned}\frac{\beta\Omega_{\rm eff}}{N}=&\frac{\beta\Omega_0}{N}+\frac{1}{N}\int_0^\beta d\tau\bar{\mathbf{j}}(\tau)\cdot\bar{\mathbf{r}}(\tau)\\&+\tfrac{1}{2}\int_0^\beta d\tau'd\tau_2\bar{\mathbf{r}}^T(\tau_2)\Gamma(\tau_2-\tau_1)\bar{\mathbf{r}}(\tau_1)\ ,\end{aligned} \tag{3.37}$$

where a source term has been added to enable us to generate the Bose propagator from the partition function. Carrying out the path integral over the Gaussian fluctuations, we find

$$Z_{\rm MV}[\bar{\mathbf{j}}]=e^{-\beta(\Omega_0+\Omega_1)}\exp\left[\frac{1}{2N}\int_0^\beta d\tau_1d\tau_2\bar{\mathbf{j}}^T(\tau_2)\Gamma(\tau_2-\tau_1)^{-1}\bar{\mathbf{j}}(\tau_1)\right]\ , \tag{3.38}$$

where $\Omega_1=\frac{1}{2}k_BT\,\mathrm{Tr}\ln(N\Gamma)$. From (3.38) we can read off the Bose propagator as

$$\langle T\delta\bar{\mathbf{r}}(\tau)\delta\bar{\mathbf{r}}(0)\rangle=\frac{\delta^2\ln(Z_{\mathrm{MV}}[\bar{\mathbf{j}}])}{\delta\bar{\mathbf{j}}(\tau)\delta\bar{\mathbf{j}}(0)}\bigg|_{\bar{\mathbf{j}}=\bar{0}}=\frac{1}{N}\Gamma^{-1}(\tau)\ , \quad (3.39)$$

and from (3.26) and (3.27) we see that $\Gamma(\tau)$ is divided into two parts,

$$\Gamma(\tau)=\Gamma^{(0)}(\tau)+\Pi^{(0)}(\tau)\ , \quad (3.40)$$

where

$$\Gamma^{(0)}(\tau)=2\begin{bmatrix}\lambda_0 & 1\\ 1 & 0\end{bmatrix}\delta(\tau) \quad (3.41)$$

is the bare Bose contribution to the Gaussian terms and Π is the self-energy of the Bose field generated from the random-phase approximation (RPA) polarization graphs formed by contracting two mean-field Fermion propagators with H_{int} (Fig. 5).

We can interpret

$$\frac{1}{N}[\Gamma^{(0)}(\tau)]^{-1}=\frac{1}{N}\begin{bmatrix}0 & 1\\ 1 & -\lambda_0\end{bmatrix}\delta(\tau) \quad (3.42)$$

as the bare propagator for the Bose field, and $(1/N)\Gamma^{-1}(\tau)$ as the renormalized propagator due to the interaction with the electrons. The bare propagator (3.42) gives rise to a static interaction

$$\hat{\mathscr{H}}_{\mathrm{eff}}=\tfrac{1}{2}\tilde{U}\sum_{m,n}f_m^\dagger f_{m'}^\dagger f_{m'}f_m + \sum_{m,m',k}\gamma_k[(\delta_{mm'}-\hat{n}_{fm'})c_{km}^\dagger f_m+\mathrm{H.c.}] \quad (3.43)$$

between the electrons where $\tilde{U}=\lambda_0/(N\tilde{r}_0^2)$ and $\gamma_k=V(k)/(N\tilde{r}_0)$. The Gaussian fluctuations are simply equivalent to summing the RPA diagrams generated by this interaction (with the Hartree terms already included through the mean-field terms). Apart from the additional mixing term on the right-hand side, this effective interaction bears a great resemblence to the Anderson model with finite U. The interaction term coupling f occupation to hybridization was actually considered by Blandin, and more recently by Varma[41] in the context of large-U Anderson models.

One interesting feature of (3.43) is the *absence* of any bare Kondo spin exchange $J^*\sum_{k,m,k',m'}c_{km}^\dagger f_m f_{m'}^\dagger c_{km'}$ term between the f electrons and conduction electrons. We see that by making Newns and Read's gauge transformation we have transformed away the bare Kondo interaction that gives rise to infrared difficulties.

$\Omega=\Omega_0+\Omega_1$ can be intepreted analogously in terms of Feynman diagrams. Ω_0 is the sum of all closed-loop diagrams created by the contraction of the fermion lines with the (renormalized) hybridization H_{mix}^* and Ω_1 is the sum of one-loop Bose propagator lines formed by contracting the bare propagator $(1/N)\Gamma^{(0)-1}$ with the polarization graphs $N\Pi$ (Fig. 6). Each Bose propagator carries a factor $1/N$, while each polarization graph is $O(N)$ due to the sum over N angular momentum channels. Thus Ω_0 is $O(N)$ while Ω_1 is $O(1)$.

From the RPA diagrams we find that

$$\Pi_{rr}(\tau)=[2G_{fk}(\tau)G_{fk}(-\tau)+G_b(\tau)G_f(-\tau)+G_f(\tau)G_b(-\tau)]\ ,$$

$$\Pi_{r\dot{\theta}}(\tau)=\Pi_{\dot{\theta}r}(\tau)=(\tilde{r}_0^{-1})[G_{fk}(\tau)G_f(-\tau)+G_f(\tau)G_{fk}(-\tau)]\ , \quad (3.44)$$

$$\Pi_{\dot{\theta}\dot{\theta}}(\tau)=(\tilde{r})_0^{-2}G_f(\tau)G_f(\tau)\ ,$$

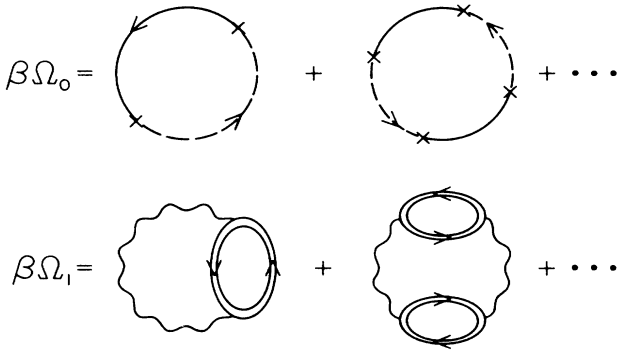

FIG. 5. The mean-field free energy $\beta\Omega_0$ and the leading Gaussian correction $\beta\Omega_1$ to the free energy, represented in diagrams. The single-dotted lines are the unhybridized f propagators, the oscillating lines represent the bare-boson propagator $[N\Gamma(0)(i\nu_n)]^{-1}$ of (3.42) and the loops with arrows in $\beta\Omega_1$ are the RPA boson self-energies $\Pi^0(i\nu_n)$.

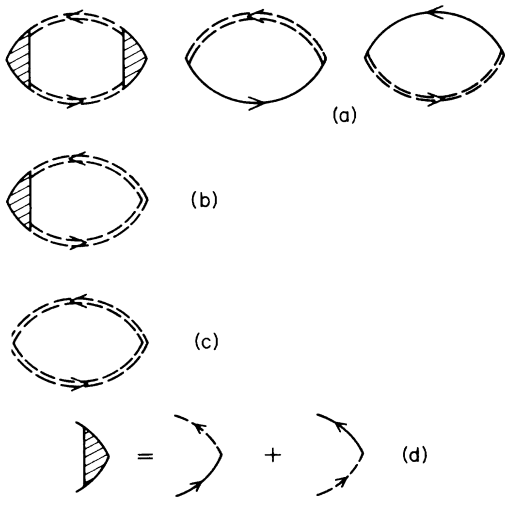

FIG. 6. RPA diagrams for the one-impurity model. A solid line denotes a conduction electron propagator, while a double-dotted line represents an f propagator with hybridization insertions. (a) Π_{rr}, (b) $\Pi_{r\dot{\theta}}$, and (c) $\Pi_{\dot{\theta}\dot{\theta}}$.

where

$$G_{fk}(\tau)=\sum_k V(k)\langle Tf_m(\tau)c^\dagger_{km}(0)\rangle ,$$
$$G_f(\tau)=\langle Tf_m(\tau)f^\dagger_m(0)\rangle ,$$

and

$$G_b(\tau)=\sum_{k,k'} V(k)V(k')\langle Tc_{km}(\tau)c^\dagger_{k'm}(0)\rangle .$$

Defining $\Pi(\tau)=\beta^{-1}\sum_n \Pi(i\nu_n)e^{-i\nu_n\tau}$ and inserting

$$G_f(i\omega_n)=[i\omega_n-\tilde{E}_f-\tilde{r}_0^2\Sigma_f(i\omega_n)]^{-1} ,$$
$$G_{fk}(i\omega_n)=\tilde{r}_0\Sigma_f(i\omega_n)G_f(i\omega_n) ,$$

and

$$G_b(i\omega_n)=\Sigma_f(i\omega_n)+\tilde{r}_0^2[\Sigma_f(i\omega_n)]^2G_f(i\omega_n)$$

for the mean-field propagators (see Sec. II C) we find

$$\Pi_{rr}(i\nu_n)=\beta^{-1}\sum_n G_f(i\omega_n+i\nu_n)G_f(i\omega_n)\times[\alpha(i\omega_n,i\nu_n)]^2+\Gamma(i\nu_n) ,$$
$$\Pi_{r\dot{\theta}}(i\nu_n)=(\beta\tilde{r}_0)^{-2}\sum_n G_f(i\omega_n+i\nu_n)G_f(i\omega_n)\times\alpha(i\omega_n,i\nu_n) , \quad (3.45)$$
$$\Pi_{\dot{\theta}\dot{\theta}}(i\nu_n)=(\beta\tilde{r}_0^2)^{-1}\sum_n G_f(i\omega_n+i\nu_n)G_f(i\omega_n) ,$$

where $\alpha(i\omega_n,i\nu_n)=\tilde{r}_0[\Sigma_f(i\omega_n)+\Sigma_f(i\omega_n+i\nu_n)]$ and

$$\Gamma(i\nu_n)=\beta^{-1}\sum_n G_f(i\omega_n)[\Sigma_f(i\omega_n+i\nu_n)-\Sigma_f(i\omega_n-i\nu_n)] . \quad (3.46)$$

Using the large bandwidth approximation introduced in Sec. I, we find (Appendix A)

$$\Pi_{rr}(i\nu_n)=2\left\{\frac{1}{g(i\nu_n)}\mathrm{Re}\mathscr{L}(i\nu_n)+\frac{\Delta}{\pi}\left[\mathrm{Re}\tilde{\psi}(\xi)-\ln\left|\frac{D\beta}{2\pi}\right|\right]\right\} ,$$
$$\Pi_{r\dot{\theta}}(i\nu_n)=2\frac{1}{\nu_n}\mathrm{Im}\mathscr{L}(i\nu_n)-2 , \quad (3.47)$$
$$\Pi_{\dot{\theta}\dot{\theta}}(i\nu_n)=-2\left[\frac{g(i\nu_n)}{\nu_n^2}\right]\mathrm{Re}\mathscr{L}(i\nu_n) \quad (n>0) ,$$

where $\Pi(i\nu_n)=\Pi^*(-i\nu_n)$ for $n<0$ and

$$g(i\nu_n)=\frac{i\nu_n}{i\nu_n+2i\tilde{\Delta}} ,$$
$$\mathscr{L}(i\nu_n)=\Delta/\pi[\tilde{\psi}(\xi+i\nu_n)-\tilde{\psi}(\xi)]+i\nu_n , \quad (3.48)$$

where $\tilde{\psi}(z)=\psi(\frac{1}{2}+z\beta/2\pi i)$ as before. This becomes

$$\mathscr{L}(i\nu_n)=\frac{\Delta}{\pi}\ln\left[\frac{\xi+i\nu_n}{\xi}\right]+i\nu_n \quad (3.49)$$

in the $T\to 0$ limit. Summing $\Gamma^{(0)}$ and Π together now gives

$$\Gamma(i\nu_n)=2\begin{bmatrix}\frac{1}{g(i\nu_n)}\mathrm{Re}\mathscr{L}(i\nu_n) & \frac{1}{\nu_n}\mathrm{Im}\mathscr{L}(i\nu_n)\\ \frac{1}{\nu_n}\mathrm{Im}\mathscr{L}(i\nu_n) & \frac{-g(i\nu_n)}{\nu_n^2}\mathrm{Re}\mathscr{L}(i\nu_n)\end{bmatrix}+2\begin{bmatrix}\lambda+\frac{\Delta}{\pi}\left[\mathrm{Re}\tilde{\psi}(\xi)-\ln\left|\frac{D\beta}{2\pi}\right|\right] & 0\\ 0 & 0\end{bmatrix} , \quad (3.50)$$

where the second term vanishes at the saddle point. Inverting this expression yields

$$\Gamma^{-1}(i\nu_n)=R(i\nu_n)=\frac{1}{2\mathscr{L}(i\nu_n)\mathscr{L}^*(i\nu_n)}\begin{bmatrix}g(i\nu_n)\mathrm{Re}\mathscr{L}(i\nu_n) & \nu_n\mathrm{Im}\mathscr{L}(i\nu_n)\\ \nu_n\mathrm{Im}\mathscr{L}(i\nu_n) & -[\nu_n^2/g(i\nu_n)]\mathrm{Re}\mathscr{L}(i\nu_n)\end{bmatrix} . \quad (3.51)$$

Appendix (B) shows how equivalent results can be obtained using the Cartesian-Bose coordinates, where one finds (choosing $\tilde{b}_0=\tilde{r}_0$, $\delta\tilde{b}=b_x+ib_y$)

$$\begin{bmatrix}\langle b_x(i\nu_n)b_x(-i\nu_n)\rangle & -i\langle b_x(i\nu_n)b_y(-i\nu_n)\rangle\\ i\langle b_y(i\nu_n)b_x(-i\nu_n)\rangle & \langle b_y(i\nu_n)b_y(-i\nu_n)\rangle\end{bmatrix}=\frac{1}{N}\begin{bmatrix}R_{rr}(i\nu_n) & \frac{-1}{i\nu_n}R_{r\dot{\theta}}(i\nu_n)\\ -\frac{R_{r\dot{\theta}}(i\nu_n)}{i\nu_n} & -\frac{1}{\nu_n^2}R_{\dot{\theta}\dot{\theta}}(i\nu_n)\end{bmatrix} . \quad (3.52)$$

The frequency denominator present in $\langle b_y(i\nu_n)b_y(-i\nu_n)\rangle$ is the zero-mode divergence associated with the low-frequency spin fluctuations.

In the Kondo regime, the first term in $\mathscr{L}(i\nu_n)$ dominates and provided one is interested in properties at frequencies $\nu\ll\Delta$, the linear frequency term can be neglected. We can analytically extend these results to the real axis, for instance the radial propagator is given by

$$\langle\delta\tilde{r}(\nu+i\delta)\delta\tilde{r}(\nu+i\delta)\rangle=\frac{1}{4Ng(\nu)}\left[\frac{1}{\mathscr{L}(\nu)}+\frac{1}{\mathscr{L}^*(\nu)}\right] , \quad (3.53)$$

$$\mathscr{L}^*(\nu)=\frac{\Delta}{\pi}[\tilde{\psi}(\nu-\tilde{\xi})-\tilde{\psi}(-\xi^*)]-\nu .$$

We shall show that this quantity is proportional to the

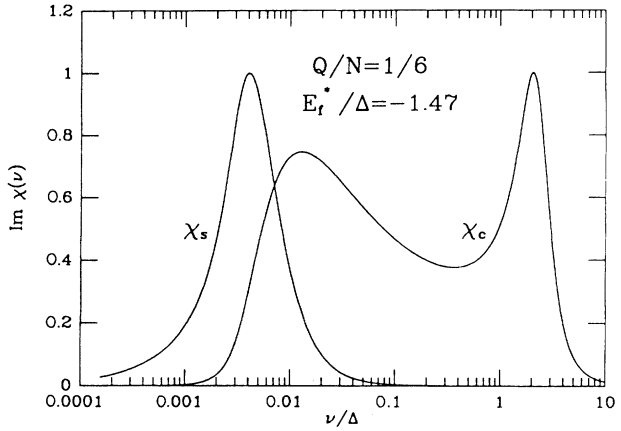

FIG. 7. The imaginary parts of the spin and charge susceptibilities, plotted on a logarithmic axis for $E_f^*/\Delta=-1.47$ and $Q/N=\frac{1}{6}$. The y axis scale is arbitrary, and adjusted to give the same peak heights. Spin fluctuations are concentrated at energies around the Kondo temperature, whilst charge fluctuations span a broad range of frequencies and are peaked at the energy E_q defined in Sec. III F.

dynamic charge susceptibility $\chi_c(\nu)$, which is plotted in Fig. 7. The bulk of the radial oscillations occur at a much higher frequency $\sim E_f^*$ than the renormalized resonant level width $\tilde{\Delta}$. We shall see that we can associate these fluctuations with the high-frequency charge fluctuations. At low temperature the quasiparticles move in the average field of the Boson, and we fail to see these high-frequency fluctuations.

From $\Gamma(i\nu_n)$ we can also determine the shift in the free energy due to zero-point and thermal fluctuations

$$\Omega_1=k_BT\,\mathrm{Re}\sum_{n>0}\ln\left[\frac{2\mathscr{L}(i\nu_n)}{i\nu_n}\right]=\int_{-\infty}^{+\infty}\frac{d\nu}{\pi}[n(\nu)+\tfrac{1}{2}]\mathrm{Im}\left[\ln\left[\frac{\mathscr{L}(\nu)}{\nu}\right]\right]. \tag{3.54}$$

We shall later use the renormalized free energy to calculate the effect of the fluctuations on the saddle point.

D. Dynamic susceptibilities

The collective properties of the Fermi liquid are related to the Bose fluctuations. In this section we relate the dynamic correlations in the spin, charge, and $q(\tau)=Q(\tau)/N$ to the Gaussian fluctuations.

To determine the collective spin and charge fluctuations of the f electrons we associate a source term with the f occupations which we add to the free-energy functional:

$$\beta F_s[\phi_m]=\sum_{m=-j}^{j}\int_0^\beta d\tau\,\phi_m(\tau)n_{fm}(\tau)\,, \tag{3.55}$$

which enables the determination of the dynamic susceptibility of the f electrons from a functional derivative of the full free energy

$$\chi_{mm'}(\tau)=\langle T\delta\hat{n}_{fm}(\tau)\delta\hat{n}_{fm'}(0)\rangle=\frac{\delta^2\ln Z_{\mathrm{MV}}[\phi]}{\delta\phi_m(\tau)\delta\phi_{m'}(0)}\,. \tag{3.56}$$

Diagrammatically this is simply the RPA susceptibility. With the source term (3.55), F_Ψ now takes the form

$$\beta F_\psi[\bar{\mathbf{r}},\phi_m]=\sum_m\mathrm{Tr}_\tau\ln\{G_f^{(0)}(\tau-\tau')+r(\tau)\Sigma_f^0(\tau-\tau')r(\tau')+[i\dot{\theta}(\tau)+\phi_m(\tau)]\hat{n}_{fm}(\tau)\} \tag{3.57}$$

and the source current enters identically to the angular velocity. Thus to second order the effective free energy is given by

$$\beta\Omega_{\mathrm{eff}}=\beta\Omega_0+\frac{N}{2}\bar{\mathbf{r}}^T\cdot\Gamma^{(0)}\cdot\bar{\mathbf{r}}+\tfrac{1}{2}\sum_m(\bar{\mathbf{r}}+\bar{\boldsymbol{\phi}}_m)^T\Pi(\bar{\mathbf{r}}+\bar{\boldsymbol{\phi}}_m)+(\bar{\mathbf{j}}\cdot\bar{\mathbf{r}})\,, \tag{3.58}$$

where we have used a shorthand notation for the time integrations $(\bar{\mathbf{j}}\cdot\bar{\mathbf{r}})=\int_0^\beta d\tau\,\bar{\mathbf{j}}(\tau)\cdot\bar{\mathbf{r}}(\tau)$ and set $\bar{\boldsymbol{\phi}}_m=(0,\tilde{r}_0\phi_m)$. The Gaussian integral over the Bose fields then yields

$$\ln(Z_{\mathrm{MV}}[\bar{\mathbf{j}},\phi_m])=-\beta(\Omega_0+\Omega_1)+\frac{1}{2N}\left[\bar{\mathbf{j}}+\Pi\sum_m\bar{\boldsymbol{\phi}}_m\right]^T\Gamma^{-1}\left[\bar{\mathbf{j}}+\Pi\sum_m\bar{\boldsymbol{\phi}}_m\right]-\sum_m\bar{\boldsymbol{\phi}}_m^T\Pi\bar{\boldsymbol{\phi}}_m\,, \tag{3.59}$$

so that

$$\chi_{mm'}=\tilde{r}_0^2\left[\frac{1}{N}(\Pi\Gamma^{-1}\Pi)-\delta_{mm'}\Pi\right]_{\dot{\theta}\dot{\theta}}, \tag{3.60}$$

where $\dot{\theta}\dot{\theta}$ denotes the $(i\tilde{r}_0\dot{\theta},i\tilde{r}_0\dot{\theta})$ element of the matrix operator. In frequency space with

$$\chi_{mm'}(\tau)=\beta^{-1}\textstyle\sum_{i\nu_n}\chi_{mm'}(i\nu_n)e^{-i\nu_n\tau}$$

we write

$$\chi_{mm'}(i\nu_n)=\tilde{r}_0^2\left[\frac{1}{N}\Pi(i\nu_n)\Gamma^{-1}(i\nu_n)\Pi(i\nu_n)-\delta_{mm'}\Pi(i\nu_n)\right]_{\dot{\theta}\dot{\theta}}. \tag{3.61}$$

It is now straightforward to derive the spin and charge susceptibilities

$$\chi_s(\tau)=\langle TM_z(\tau)M_z(0)\rangle\,,\qquad\chi_c(\tau)=\langle T\delta\hat{n}_f(\tau)\delta\hat{n}_f(0)\rangle\,, \tag{3.62}$$

where $M_z=\sum_{f,m}mn_{fm}$. Setting $\chi_s=\sum_m m^2\tilde{\chi}_s$ and $\chi_c=N\tilde{\chi}_c$ we find

$$\begin{aligned}\tilde{\chi}_c(i\nu_n)&=\tilde{r}_0^2[\Pi(i\nu_n)\Gamma^{-1}(i\nu_n)\Pi(i\nu_n)-\Pi(i\nu_n)]_{\dot{\theta}\dot{\theta}}\\&=\tilde{r}_0^2[\Gamma^{(0)}(i\nu_n)\Gamma^{-1}(i\nu_n)\Gamma^{(0)}(i\nu_n)]_{\dot{\theta}\dot{\theta}}\\&=N[4\tilde{r}_0^2\langle\delta r(i\nu_n)\delta r(i\nu_n)\rangle]\\&=2r_0^2g(i\nu_n)\mathrm{Re}[\mathscr{L}(i\nu_n)^{-1}]\,,\end{aligned} \tag{3.63}$$

while

$$\tilde{\chi}_s(i\nu_n) = -\tilde{r}_0^2[\Pi(i\nu_n)]_{\dot{\theta}\dot{\theta}} = \left[\frac{2\tilde{r}_0^2}{(\nu_n+2\tilde{\Delta})\nu_n}\right]\mathrm{Re}\mathscr{L}(i\nu_n) \tag{3.64}$$

which is plotted in Figs. 7 and 8. Taking $i\nu_n \to 0$ we find that the static susceptibilities are

$$\tilde{\chi}_c(0) = \frac{1}{\Delta}\mathrm{Re}\left[1+\frac{\Delta}{\pi}\tilde{\psi}'(\xi)\right]^{-1}, \qquad \tilde{\chi}_s(0) = -\mathrm{Im}\left[\frac{1}{\pi}\tilde{\psi}'(\xi)\right], \tag{3.65}$$

which are the results obtained more directly in Sec. II. Analytically extending the spin susceptibility to the real axis, we find

$$\tilde{\chi}_s(\nu+i\delta) = \frac{-1}{(\nu+2i\tilde{\Delta})\nu}\frac{\tilde{\Delta}}{\pi}[\tilde{\psi}(\xi+\nu)+\tilde{\psi}(\nu-\tilde{\xi}) -\tilde{\psi}(\xi)-\tilde{\psi}(-\xi^*)], \tag{3.66}$$

which at zero temperature yields

$$\tilde{\chi}_s(\nu+i\delta) = \frac{-1}{(\nu+2i\tilde{\Delta})\nu}\frac{\tilde{\Delta}}{\pi}\left[\ln\left[\frac{(\xi+\nu)(\xi^*-\nu)}{\xi\xi^*}\right]\right]. \tag{3.67}$$

Taking the $\nu \to 0$ limit, we find

$$\lim_{\nu\to 0}\mathrm{Im}\frac{\chi_s(\nu+i\delta)}{\nu} = \pi\left[\frac{\tilde{\Delta}}{\pi(\tilde{E}_f^2+\tilde{\Delta}^2)}\right]^2 = \pi[\tilde{\chi}_s(0,T=0)]^2 . \tag{3.68}$$

This is the Korringa relation derived by Shiba for the infinite-U Anderson model.[42] The satisfaction of this equality in our leading fluctuations is an indication that our approximation is conserving the Ward identities associated with spin conservation. Earlier work found difficulties[10] in eliminating infrared divergences at zero frequency and failed to satisfy this relationship.

From the relations (3.63) and (3.64) we note that we can write the spin and charge susceptibilities in an alternate form

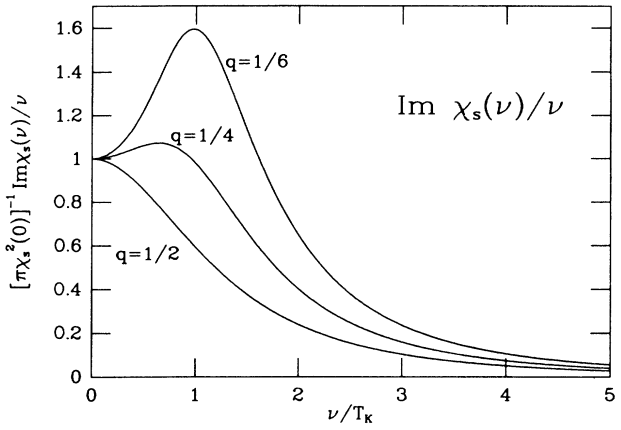

FIG. 8. Dynamic spin susceptibility $\mathrm{Im}\tilde{\chi}(\nu)/\nu$ for the cases $q=\frac{1}{2}$, $\frac{1}{4}$, and $\frac{1}{6}$, in the Kondo regime $n_f/Q=0.95$.

$$\bar{\chi}_s(\tau) = \frac{\delta^2\beta\Omega_{\mathrm{eff}}[\bar{\mathbf{r}}]}{\delta\dot{\theta}(\tau)\delta\dot{\theta}(0)}, \qquad \tilde{\chi}_c(\tau) = N\langle\delta\tilde{r}^2(\tau)\delta\tilde{r}^2(0)\rangle . \tag{3.69}$$

The relationship between the spin susceptibility and angular stiffness is one we expect to be preserved when higher-order corrections are added to the polarization diagrams. The second relationship links the charge fluctuations to the radial fluctuations and is a consequence of the Q conservation.

From (3.59) we can also calculate the correlation between the radial fluctuations and the charge fluctuations

$$\langle T\delta\tilde{r}(\tau)\delta\hat{n}_{fm}(0)\rangle = \frac{\delta^2\ln Z[\bar{\mathbf{j}},\phi_m]}{\delta j_r(\tau)\delta\phi_m(0)} = -2\tilde{r}_0\langle\delta\tilde{r}(\tau)\delta\tilde{r}(0)\rangle , \qquad -2\tilde{r}_0\langle T\delta\tilde{n}_f(\tau)\delta\tilde{r}(0)\rangle = \langle T\delta\tilde{n}_f\delta\tilde{n}_f(0)\rangle , \tag{3.70}$$

where $\tilde{n}_f = n_f/N$, from which we see they are anticorrelated. We can sum all these fluctuations to determine the fluctuations in $q(\tau)$.

$$\langle T\delta q(\tau)\delta q(0)\rangle = 4\tilde{r}_0^2\langle\delta\tilde{r}(\tau)\delta\tilde{r}(0)\rangle + 2\tilde{r}_0\langle\delta\tilde{r}(\tau)\delta\tilde{n}_f(0)\rangle + 2\tilde{r}_0\langle\delta\tilde{n}_f(\tau)\delta\tilde{r}(0)\rangle + \langle\delta\tilde{n}_f(\tau)\delta\tilde{n}_f(0)\rangle = 0 , \tag{3.71}$$

and we see that the anticorrelations between the Bose and f-electron fields lead to a vanishing correlation function. This is a crucial result, for it explicitly shows that we are consistently maintaining q conservation at all times to leading order in the Gaussian fluctuations. We note that the way our constraint is built in derives from the underlying symmetry of the dynamics (see Appendix C), rather than a careful selection of time-ordered Goldstone diagrams as in perturbative schemes.[9-12]

E. Fermi-liquid properties

The low-energy static Fermi liquid properties are directly related to the Bose propagators (Fig. 9). Thus the electron part of the quasiparticle interactions is given by

$$\mathscr{H}_{\mathrm{int}} = \tfrac{1}{2}U^*\sum_{m,m'} f_m^\dagger f_{m'}^\dagger f_{m'} f_m , \tag{3.72}$$

where

$$U^* = -\langle i\dot{\theta}(\nu=0)i\dot{\theta}(\nu=0)\rangle = -\frac{1}{Nr_0^2}R_{\dot{\theta}\dot{\theta}}(\nu=0) = \frac{1}{N}\pi\tilde{\Delta}\mathrm{Im}\left[\pi\tilde{r}_0^2+\frac{\tilde{\Delta}}{\xi}\right]^{-1} \underset{\tilde{\Delta}\to 0}{\to} \frac{1}{N}\pi\tilde{\Delta} \tag{3.73}$$

is the renormalized interaction strength. By summing up

the interaction terms generated from each component of $\mathbf{R}(0)$ (Fig. 10) we can determine the net interactions between the quasiparticles. This is most simply done in the following more physical fashion. Suppose we add an additional quasiparticle to a conduction band state at the Fermi energy. This particle has energy $\mu-\Delta\varepsilon_k(\delta/\pi)$, where $\Delta\varepsilon_k$ is the spacing of conduction band states and $\delta_f=\tan^{-1}(\tilde{\Delta}/\tilde{E}_f)$ is the scattering phase shift at the Fermi surface. The second term is the depression of the conduction electron energy due to the impurity. Setting $(\Delta\varepsilon_k)^{-1}=\rho$, the conduction band density of states, then by adding the quasiparticle we increase the free energy of the system by the infinitesimal amount

$$\delta E_0=-\frac{1}{\pi\rho}\delta_f \ . \tag{3.74}$$

We can write this term as $\delta E_0=\mathrm{Im}[\delta E_c(\xi)]$, where $\delta E_c(\xi)=-(\pi\rho)^{-1}\ln(\xi)$. Now using the results of Sec. II we can write the total energy of the system as $E_0=\mathrm{Im}[NE_c(\xi)+\delta E_c(\xi)]$ where

$$E_c(\xi)=\frac{(\xi-E_c^*)^2}{2\Delta}+\frac{\xi}{\pi}\ln\left[\frac{\xi\pi}{\Delta}\right] \ . \tag{3.75}$$

We can calculate the shift $d\xi$ in ξ from its saddle point value by reminimizing $E_c+\delta E_c$ with respect to ξ. This yields

$$d\xi=\frac{1}{N\rho}\left[1+\frac{\pi\xi}{\Delta}\right]^{-1} \tag{3.76}$$

from which we deduce that the shift in the scattering phase shift at the Fermi energy due to the presence of the additional quasiparticle is

$$\frac{d\delta_{fm}}{\delta n_{m'}}=\Phi=\frac{1}{N\rho}\mathrm{Im}\left[\xi\left[1+\frac{\pi\xi}{\Delta}\right]\right]^{-1}, \quad m\neq m' \ . \tag{3.77}$$

If we expand $\delta(\varepsilon)$ about the Fermi energy we find

$$\delta_f(\varepsilon)=\delta_0+\pi\rho_f\varepsilon+\sum_{m(\neq m')}\Phi\delta n_{m'} \ , \tag{3.78}$$

where

$$\rho_f=\frac{1}{\pi}\frac{\tilde{\Delta}}{(\tilde{\Delta}^2+\tilde{E}_f^2)}$$

and the condition $m\neq m'$ arises from the cancellation of direct exchange terms in the interaction for the case of identical spins. This leading order result has the same form as the Nozières-Fermi liquid picture of a Kondo impurity.[6] We can actually take the Kondo limit by taking $\tilde{\Delta}\ll\Delta$, leading to $\Phi\approx(1/N_\rho)\mathrm{Im}\xi^{-1}$, so that in this limit

$$N\Phi\rho=-\pi\rho_f \ , \tag{3.79}$$

which is the Nozières-Fermi liquid identity written to leading order in $1/N$.

For the single impurity this calculation merely serves as an exercise in demonstrating the consistency of our calculational procedure with the known Fermi-liquid picture. Its full value will emerge when we extend this calculation to more than one impurity where the additional degrees of freedom prevent us from deducing the Fermi-liquid properties from qualitative arguments.

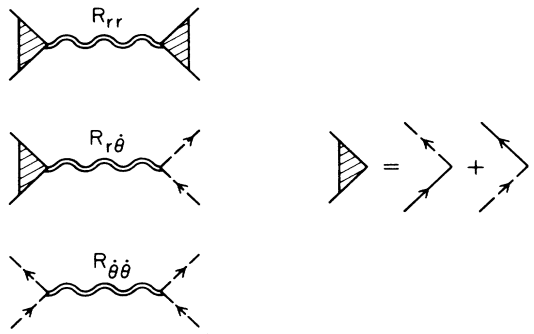

FIG. 9. Showing the interactions that are propagated by the Bose fluctuations.

F. High- and low-energy behavior of fluctuations

In this section we wish to show how the fluctuations at high frequencies reproduce the known weak coupling properties of the infinite-U Anderson model, and also study how, in the conventional picture, the Kondo interaction scales to strong coupling. To carry out this discussion, we will consider the normal Bose propagator $\langle Tb(\tau)b^\dagger(0)\rangle$, reintroducing the zero mode, by transforming the results we have already obtained to the Cartesian gauge.

Our interest in the Bose propagator stems from the fact that if we integrate out the Bose fluctuations, this gives rise to an interaction between the electrons of the form

$$\beta\hat{H}_i=-\frac{1}{N}\int_0^\beta d\tau'\hat{\sigma}^\dagger(\tau)J(\tau-\tau')\hat{\sigma}(\tau')+O\left[\frac{1}{N^2}\right] \ , \tag{3.80}$$

where $\hat{\sigma}(\tau)=\sum_{k,m}c_{km}^\dagger(\tau)f_m(\tau)$ as before and

$$J(\tau)=V^2\langle Tb(\tau)b^\dagger(0)\rangle \tag{3.81}$$

should be considered as a time-dependent Kondo interaction. We shall now compute the frequency behavior of this interaction at low and high energies. Quite generally, we can write the Bose propagator in polar coordinates as

$$\langle Tb(\tau)b^\dagger(0)\rangle=\langle Tr(\tau)e^{i\theta(\tau)}r(0)e^{-i\theta(0)}\rangle \ . \tag{3.82}$$

The high-frequency components of the fluctuations are small, enabling us to make the linear approximation $re^{i\theta}=r_0e^{i\theta_0}+\delta r+ir_0\delta\theta$, so at high energies $|\nu_n|\gg|\xi|$,

$$\langle b(i\nu_n)b^\dagger(i\nu_n)\rangle=\left[R_{rr}(i\nu_n)-\frac{2}{i\nu_n}R_{r\dot{\theta}}(i\nu_n)-\frac{1}{\nu_n^2}R_{\dot{\theta}\dot{\theta}}(i\nu_n)\right] \ , \tag{3.83}$$

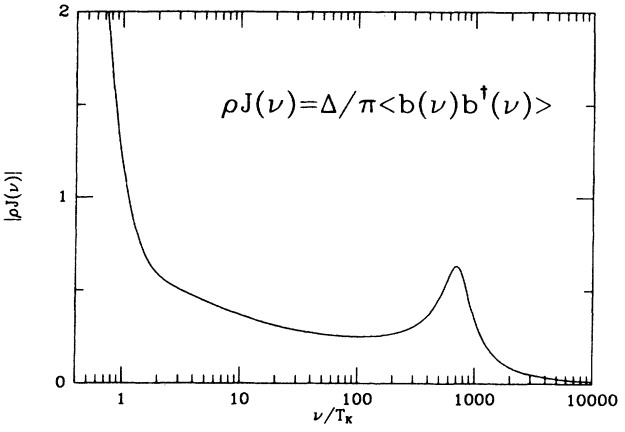

FIG. 10. The effective Kondo coupling constant, $V^2|\langle b^\dagger(\nu)b^\dagger(\nu)\rangle|$, as given by Eq. (3.83). This exhibits the qualitative properties of the Kondo interaction, namely the sudden growth at the charge fluctuation energy $E_c\sim|E_f^*|$, followed by a slow logarithmic rise as the Kondo temperature is reached, and a divergence to strong coupling at lower energies.

which is plotted in Fig. 10. Inserting the results obtained in (3.50), we find that for $|\nu|\gg|\xi|$, $g(i\nu_n)\to 1$ so that the high-frequency fluctuations have the simple form

$$\langle b(i\nu_n)b^\dagger(i\nu_n)\rangle=\frac{1}{\mathscr{L}(i\nu_n)^*}\ . \tag{3.84}$$

There are actually two energy regimes at high energies, separated by the crossover energy E_q, where $E_q+(\Delta/\pi)\ln(E_q\pi/\Delta)=|E_f^*|$.

In the "charge-fluctuation regime," $\nu>E_q$,

$$\rho J(\nu)\sim\left[\frac{\Delta}{\pi}\right]\frac{1}{\nu}\ , \tag{3.85}$$

where $J(\tau)=-\beta^{-1}\sum_n J(i\nu_n)e^{i\nu_n\tau}$. At lower energies $E_q>\nu>|\xi|$ in the spin-fluctuation regime.

$$\rho J(\nu+i\delta)\sim\frac{1}{\ln(\nu/\xi^*)} \tag{3.86}$$

which is the classic "asymptotically free" logarithmic decay of the Kondo coupling constant at high frequencies.

The crossover energy E_q was actually discovered by Haldane in his renormalization group treatment of the single impurity model.[29] Haldane scaling is equivalent to rescaling the f-level position $E_f(D')$ as the bandwidth D' is reduced, such a way as to keep the high energy invariant E_f^* (and hence the low-energy physics) constant. This leads to a rescaled f level, given by $E_f(D')=E_f+(1-1/N)(\Delta/\pi)\ln(D/D')$. When $D'=E_q$ the lower band edge becomes equal to the f-level energy $E_f(E_q)=-|E_q|$ and when the cutoff is reduced below the crossover energy, charge fluctuations become entirely virtual and they are integrated out of the rescaled Hamiltonian by a Schrieffer-Wolffe transformation to give an effective Kondo model that describes the subsequent lower-energy physics. This feature appears naturally in our semiclassical treatment of fluctuations.

At the lowest frequencies, we reach a strong coupling regime where the linear approximation to $b=re^{i\theta}$ fails because the long-time phase fluctuations are divergent. To calculate the very-long-time, low-frequency behavior of the interaction, we employ the approximation

$$\langle Tr(\tau)e^{i\theta}(\tau)r(0)e^{-i\theta(0)}\rangle\approx r_0^2\langle Te^{i\theta(\tau)-i\theta(0)}\rangle\ , \tag{3.87}$$

which determines the asymptotic behavior because the infrared divergence of the zero mode dominates the low-frequency behavior.[18]

The exponent in (3.87) can be expanded as a sum of Gaussian variables

$$\theta(\tau)-\theta(0)=\sqrt{T}\sum_n\frac{\dot\theta(i\nu_n)}{(-i\nu_n)}(e^{-i\nu_n\tau}-1) \tag{3.88}$$

and for a sum of Gaussian distributed variables A_i, $\langle\exp(\sum_i A_i)\rangle=\exp[-\frac{1}{2}\langle(\Sigma_i A_i)^2\rangle]$ using the Gaussian approximation to evaluate this correlation function, we find that

$$\langle Tb(\tau)b^\dagger(0)\rangle\sim r_0^2\exp\{-\tfrac{1}{2}\langle[\theta(\tau)-\theta(0)]^2\rangle\}\ . \tag{3.89}$$

Now we can relate the exponent to the angular velocity fluctuations

$$\tfrac{1}{2}\langle[\theta(\tau)-\theta(0)]^2\rangle=-T\sum_n\frac{\langle\dot\theta(i\nu_n)\dot\theta(-i\nu_n)\rangle}{\nu_n^2}\times(e^{-i\nu_n\tau}-1)\ , \tag{3.90}$$

where

$$\langle\dot\theta(i\nu_n)\dot\theta(-i\nu_n)\rangle=-\frac{1}{N\tilde r_0^2}R_{\dot\theta\dot\theta}(i\nu_n)\ . \tag{3.91}$$

Inserting (3.91) into (3.90) and carrying out the contour integral on the Matsubara sum then yields

$$\tfrac{1}{2}\langle[\dot\theta(\tau)-\dot\theta(0)]^2\rangle=\frac{1}{N}\int_{-\infty}^{\infty}\frac{d\nu}{\pi}[n(\nu)+1]\left[\frac{(1-e^{-\nu\tau})}{\nu^2\tilde r_0^2}\right]\mathrm{Im}R_{\dot\theta\dot\theta}(\nu+i\delta)$$

$$=\frac{1}{N}\int_0^{\infty}\frac{d\nu}{\pi}\left[\frac{(1-e^{-\nu\tau})}{\nu^2\tilde r_0^2}\right]\mathrm{Im}R_{\dot\theta\dot\theta}(\nu+i\delta)\ , \tag{3.92}$$

where the zero-temperature limit has been taken in the final equation. At low frequencies $\nu \ll \tilde{\Delta}$, $\mathrm{Im}1/\pi R_{\dot\theta\dot\theta} = \tilde{r}_0^2 \alpha \nu$ where, by direct calculation from (3.50)

$$\alpha = \lim_{\nu\to 0} \frac{R_{\dot\theta\dot\theta}}{\pi\nu\tilde{r}_0^2} = \left[\mathrm{Re}\left[\frac{\Delta}{\Delta + \pi\xi} \right] \right]^2 . \tag{3.93}$$

Consequently, at long times, at zero temperature

$$\lim_{\tau\to\infty} \langle \dot\theta(\tau)\dot\theta(0)\rangle = \frac{\alpha}{N} \ln\left[\frac{\tau}{C} \right] , \tag{3.94}$$

where C is a constant that can be determined. This leads to a power-law decay of the Kondo interaction at long times

$$\lim_{\tau\to\infty} J(\tau) = V^2 r_0^2 \left[\frac{C}{\tau} \right]^{\alpha/N} . \tag{3.95}$$

We can simply interpret the exponent of (3.95) in terms of the x-ray effect, using arguments given at the beginning of this paper by noting, from the mean-field equations that

$$\frac{dn_f}{dQ} = \mathrm{Re}\left[\frac{\Delta}{\Delta + \pi\xi} \right] , \tag{3.96}$$

so that if $\delta Q = 1$, $\delta n_f/N = (1/N) dn_f/dQ$ and there is a change in the scattering phase shift of $\Delta\delta/\pi = (1/N) dn_f/dQ$ in each channel. Thus the x-ray exponent is $N(\Delta\delta/\pi)^2 = \alpha/N$ as expected. In the case of $Q = 1$, or finite N, the change in occupation per channel is no longer an infinitesimal proportion of the occupancy, so that the full x-ray coefficient is $\alpha/N = N[\tilde{n}_f(Q) - \tilde{n}_f(Q-1)]^2$, from x-ray arguments. This result reverts to the above expression in the large N limit. In the special case of $Q = 1$, Read[39] has found $\alpha/N = n_f^2/N$ for $Q = 1$ by taking the large N limit using a different procedure, and these results are consistent with those above.

We would like to close this section by discussing the scaling properties of the interaction at low energies. Clearly, putting $\langle b(\nu) b^\dagger(\nu)\rangle = D(\nu)$, our results imply the scaling equation

$$\left[\nu \frac{\partial}{\partial\nu} + (1 - \alpha/N) \right] D(\nu) = 0 . \tag{3.97}$$

Up to order $O(1/N)$, the Kondo interaction is given by $J(\nu) = -V^2 D(\nu) + O(1/N)$, so this implies a β function

$$\beta(J) = \frac{\partial J(\nu)}{\partial \ln\nu} = -J + \frac{1}{N}, \quad J \gg 1 \tag{3.98}$$

but note that it is *incorrect* to include the additional α/N into this scaling relation, due to the $O(1/N)$ terms ignored. There are actually no further corrections, as we will now discuss.

The anomalous scaling behavior of the Bose propagator can be understood as follows. In the original Lagrangian, dimensional power counting arguments show that the slave boson is dimensionless. Assuming pure scaling of the Bose field, this would lead to a Bose propagator $\langle b(\nu) b^\dagger(\nu)\rangle = D(\nu)$ that satisfies $D(\lambda\nu) = \lambda^{-1} D(\nu)$, at low frequencies near threshold. Instead, the Bose propagator scales as $D(\lambda\nu) = \lambda^{2d}(\lambda^{-1}) D(\nu)$, where $d = \alpha/2N$, indicating that the Bose field has acquired an anomalous dimension $d = \alpha/2N$ due to the fluctuations. Now on quite general grounds, by examining the scale dependence of the Bose propagator, we expect it to satisfy[43] a Callin-Simanzik scaling equation of the form

$$\left[\nu \frac{\partial}{\partial\nu} - \tilde\beta(V) \frac{\partial}{\partial V} + [1 - 2d(V)] \right] D(\nu; V) = 0 , \tag{3.99}$$

where $\tilde\beta(V)$ is the β function for the Bose-fermion vertex V and $d(=\alpha/N)$ is the anomalous dimension of the slave boson, (defined by $d = -\frac{1}{2}\partial \ln Z_b(D)/\partial \ln D$ where Z_b is the wave-function renormalization constant of the Bose field and D is an ultraviolet cutoff). If $\tilde\beta(V)$ were nonzero, then the coupling constant V would rescale under scale transformation, and the propagator would satisfy a scaling law of the form

$$D(\lambda\nu; V) = \lambda^{-1} \exp\left[\int_1^\lambda d \ln\lambda d[V(\lambda)] \right] D[\nu, V(\lambda)] .$$

Pure power-law scaling, with no additional logarithms can only be reconciled with $\tilde\beta(V) = 0$ in strong coupling. In other words, the interaction between the slave boson and electrons *does not scale to strong coupling.*

The anomalous scaling of the Bose propagator arises from the infrared divergences about the broken symmetry starting point, and when we go to the radial gauge, the anomalous divergences are removed. The residual interaction then scales as $\sim\nu^{-1}$, so it is *constant* at long times. It is exactly this feature that gives rise to the almost-broken-symmetry feature of the Kondo ground state, for the effect of our broken-symmetry ansatz is to induce time invariant interactions that generate the heavy Fermi liquid for the general many-site case.

From this point of view, the strong-coupling effects in the original Kondo problem can be attributed to the zero mode of the Bose field. Once this zero mode is correctly taken into account by our broken-symmetry ansatz, the residual interactions are necessarily finite [$\tilde\beta(V) = 0$].

G. Full f-Green's function

The full f-electron Green's function

$$\mathcal{G}_f(\tau) = \langle T X_{0m}(\tau) X_{m0}(0)\rangle \tag{3.100}$$

contains information about both the low- and the high-frequency charge fluctuations. $\mathcal{G}_f$ determines the t matrix for scattering band electrons

$$t_{kk'}(\omega) = \frac{1}{N} V(k) V(k') \mathcal{G}_f(\omega) . \tag{3.101}$$

In the notation of the generalized Anderson model

$$\begin{aligned} \mathcal{G}_f(\tau) &= \langle T b^\dagger(\tau) f_m(\tau) f_m^\dagger(0) b(0)\rangle \\ &= \langle T r(\tau) f_m(\tau) f_m^\dagger(0) r(0)\rangle \end{aligned} \tag{3.102}$$

in the two gauges. To leading order in the fluctuations we then find

$$\frac{1}{N}\mathcal{G}_f(\tau)=\tilde{r}_0^2\langle Tf_m(\tau)f_m^\dagger(0)\rangle+\tilde{r}_0[\langle T\delta\tilde{r}(\tau)f_m(\tau)f_m^\dagger(0)\rangle+\langle Tf_m(\tau)f_m^\dagger(0)\delta\tilde{r}(0)\rangle]+\langle T\delta r(\tau)\delta r(0)f_m(\tau)f_m^\dagger(0)\rangle\ . \tag{3.103}$$

The easiest way of computing the various contributions is diagramatically. As we are only interested in the leading effects of the Gaussian fluctuations, no more than one (fully clothed) Bose propagator $(1/N)R$ appears in a graph, avoiding vertex corrections. Nevertheless, this calculation is different in a most important fashion from more conventional perturbation schemes,[9-12] for although both do not involve vertex corrections, this scheme incorporates the singular behavior of the fluctuations at low temperature by including the broken-symmetry hybridization terms. The infrared divergences associated with the zero mode have been factored away and there is no singular behavior associated with any of the gauge transformed propagators.

The Bose propagators are symmetric in time enabling so that the second and third terms in (3.103) are equal. To leading order in the fluctuations we can factorize the fourth term in (3.103) giving

$$\begin{aligned}\frac{1}{N}\mathcal{G}_f(\tau)=&\tilde{r}_0^2\langle Tf_m(\tau)f_m^\dagger(0)\rangle\\&+2\tilde{r}_0\langle T\delta r(\tau)f_m(\tau)f_m^\dagger(0)\rangle\\&+\langle\delta\tilde{r}(\tau)\delta\tilde{r}(0)\rangle\langle Tf_m(\tau)f_m^\dagger(0)\rangle\ .\end{aligned}\tag{3.104}$$

To leading order in $1/N$, the last term is $(1/N)R_{rr}(\tau)G_f^{(0)}(\tau)$, where $G_f^{(0)}(\tau)$ is the quasiparticle f propagator evaluated in mean-field theory.

The first two terms in (3.104) are simplified by an observation that provided the charge fluctuation scale $\sim|E_f^*|$ is much greater than spin fluctuation temperature $T_K=(\tilde{\Delta}^2+\tilde{E}_f^2)^{1/2}$, phase fluctuations dominate the high-energy scattering of the quasiparticles. This can be seen as follows. These terms involve frequency convolutions with fluctuation propagators $R_{\alpha\beta}(\nu)$ where the dominant contributions come from high-energy fluctuations with frequencies $|\nu|\sim|E_f^*|\gg T_K$. For the amplitude fluctuations $\delta\tilde{r}$, the vertex for coupling to f-electron lines involves an intermediate conduction electron propagator, and is $\sim\mathrm{sgn}\nu_n\tilde{\Delta}/\tilde{r}_0$ for $\nu_n\gg\tilde{\Delta}$. Phase velocity fluctuations $i\tilde{r}_0\theta$ couple to the f-electron line with coupling $1/\tilde{r}_0$, and since each time derivative associated with the phase velocity contributes a factor $i\nu_n$, the overall coupling of a transverse fluctuation $i\tilde{r}_0\delta\theta$ to an f-electron line is $O(i\nu_n/\tilde{r}_0)$. The typical frequency of the high-energy contribution is $|\nu|\sim O(E_f^*)$, thus scattering from high-frequency phase fluctuations is $O(|E_f^*|/\tilde{\Delta})$ larger than the corresponding amplitude fluctuations. This enables us to make the approximations

$$\begin{aligned}\tilde{r}_0\langle Tf_m(\tau)f_m^\dagger(0)\rangle_{i\omega_n}&=\tilde{r}_0^2G_f^{(0)}(i\omega_n)+\frac{1}{N}[G_f^{(0)}(i\omega_n)]^2\Sigma_{\dot\theta\dot\theta}(i\omega_n)+O\left(\frac{\tilde{\Delta}}{N|E_f^*|},\frac{1}{N^2}\right),\\ \tilde{r}_0\langle T\delta\tilde{r}(\tau)f_m(\tau)f_m^\dagger(0)\rangle_{i\omega_n}&=\frac{1}{N}G_f^{(0)}(i\omega_n)\Sigma_{r\dot\theta}(i\omega_n)+O\left(\frac{\tilde{\Delta}}{N|E_f^*|},\frac{1}{N^2}\right).\end{aligned}\tag{3.105}$$

Here $(1/N)\Sigma_{\alpha\beta}(i\omega_n)$ denotes a self-energy for scattering off fluctuations, given by

$$\Sigma_{\alpha\beta}(i\omega_n)=\frac{1}{\beta}\sum_{i\nu_n}R_{\alpha\beta}(i\nu_n)G_f^{(0)}(i\omega_n-i\nu_n)\ . \tag{3.106}$$

We can summarize these results by writing

$$\mathcal{G}(i\omega_n)=(N\tilde{r}_0^2)G_f^{(0)}(i\omega_n)+\{[G_f^{(0)}(i\omega_n)]^2\Sigma_{\dot\theta\dot\theta}(i\omega_n)+2G_f^{(0)}(i\omega_n)\Sigma_{\dot\theta r}(i\omega_n)+\Sigma_{rr}(i\omega_n)\}\ . \tag{3.107}$$

The first term is merely the quasiparticle resonance, with renormalization constant $Z_f=N\tilde{r}_0^2$, while the second terms come from fluctuations in the renormalized potential that scatters conduction electrons.

Carrying out the Matsubara frequency sum in (3.106) gives

$$\Sigma_{\alpha\beta}(\omega)=\int\frac{d\omega'}{\pi}\frac{1}{(\omega-\omega')}\mathrm{Im}\Sigma_{\alpha\beta}(\omega-i\delta)\ , \tag{3.108}$$

where

$$\begin{aligned}\mathrm{Im}\Sigma_{\alpha\beta}(\omega-i\delta)=\int\frac{d\nu}{\pi}&[1+n(\nu)-f(\omega-\nu)]\\&\times\mathrm{Im}G_f^{(0)}(\omega-\nu-i\delta)\\&\times\mathrm{Im}R_{\alpha\beta}(\nu+i\delta)\ .\end{aligned}\tag{3.109}$$

Now the fluctuations in the Bose field are spread over a much broader energy range than the Kondo resonance, and at zero temperature this enables us to approximate this integral by

$$\mathrm{Im}\Sigma_{\alpha\beta}(\omega-i\delta)=[\delta(\omega)/\pi-\tilde{n}_f]\mathrm{Im}R_{\alpha\beta}(\omega+i\delta)\qquad(|\omega|>T)\ , \tag{3.110}$$

where $\delta(\omega)=\tan^{-1}[\tilde{\Delta}/(\tilde{E}_f-\omega)]$ is the energy-dependent phase shift of the Kondo resonance referred to in preceding sections.

Provided that we are not interested in the fine structure of the Kondo resonance, then we can approximate the imaginary part of $\mathcal{G}_f(\omega)$ by ignoring the real parts of $\Sigma_{\alpha\beta}$, which enables us to write down a closed form expression for the full f-electron Green's function at $T=0$,

$$\mathrm{Im}\mathcal{G}_f(\omega-i\delta)=N\tilde{r}_0^2\left[\frac{\tilde{\Delta}}{(\omega-\tilde{E}_f)^2+\tilde{\Delta}^2}\right]$$
$$+\frac{1}{\pi}([\delta(\omega)-\delta(0)]\{\mathrm{Im}R_{rr}(\omega+i\delta)+2\,\mathrm{Re}G_f^{(0)}(\omega)\mathrm{Im}R_{r\dot{\theta}}(\omega+i\delta)+\mathrm{Re}[G_f^{(0)}(\omega)]^2\mathrm{Im}R_{\dot{\theta}\dot{\theta}}(\omega+i\delta)\})\ . \tag{3.111}$$

We show an example curve of this result in Fig. 11. Extending this result to finite temperature requires a more careful evaluation of the self-energies $\Sigma_{\alpha\beta}$. What is interesting about this result is that by including the fluctuations about the mean-field theory we have recovered the high-frequency spectral weight of the f state. The calculation has not entailed any numerical techniques, nor does it suffer from awkward low-energy anomalies in the spectral function.[8,24]

H. Renormalization of fluctuations and transition to weak coupling

Having computed the fluctuations about mean-field theory, it is of particular interest to examine how the saddle point position is modified when we include the $O(1/N)$ zero point and thermal fluctuations into the free-energy functional. Read[21] has examined these renormalization effects for the single-impurity-Kondo and generalized Anderson model at zero temperature, placing $Q=1/N$ before commencing the $1/N$ expansion. We wish to extend his analysis to finite temperature and all values of Q/N, to examine the full structure of the theory.

Returning to (3.54), we see that we can combine it with the mean-field free-energy function to write a full free-energy function

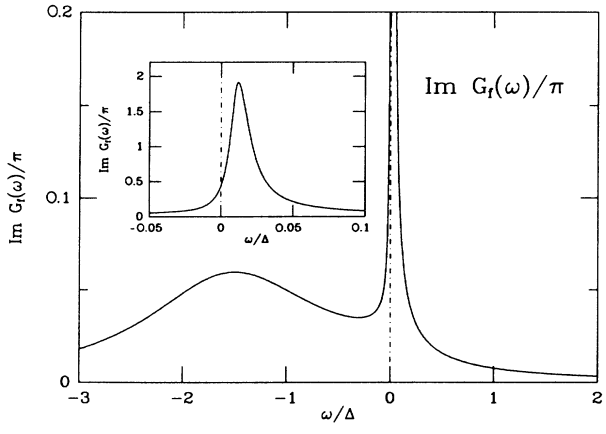

FIG. 11. The full f electron Green's function $\mathrm{Im}\mathcal{G}_f(\omega-i\delta)$ as given in (3.109), for $T=0$, $N=6$, $E_f^*/\Delta=-0.656$, $n_f/N=0.15$, and $Q/N=\frac{1}{6}$. Inset shows the asymmetric nature of the Kondo resonance.

$$\Omega=N\,\mathrm{Im}\Omega_c(\xi)\ , \tag{3.112}$$
$$\Omega_c(\xi)=\Omega_c^{\mathrm{ME}}(\xi)+\frac{1}{N}\int_{-\infty}^{\infty}\frac{d\nu}{\pi}[n(\nu)+\tfrac{1}{2}]\ln\left[\frac{\mathscr{L}(\nu)}{\nu}\right]$$

where $\Omega_c^{\mathrm{MF}}(\xi)$ is the mean-field free-energy function determined in (2.56). Now by taking the derivative with respect to ξ we find that the renormalized saddle-point condition can be written as

$$\xi-E_f^*+\frac{\Delta}{\pi}\left[\tilde{\psi}(\xi)-\ln\left[\frac{\Delta\beta}{2\pi^2 i}\right]\right]+\frac{\Delta}{N\pi}\tilde{\psi}'(\xi)\Phi(\xi,T)=0\ , \tag{3.113}$$

where we have defined

$$\Phi(\xi,T)=\Delta\int_{-\infty}^{\infty}\frac{d\nu}{\pi}[n(\nu)+\tfrac{1}{2}]\left[\frac{\tilde{\psi}'(\xi+\nu)}{\tilde{\psi}'(\xi)}-1\right]\mathscr{L}^{-1}(\nu)\ . \tag{3.114}$$

At high frequencies, governed by charge fluctuations, $\mathscr{L}(\nu)\sim\nu$, and consequently, the high-frequency charge fluctuations contribute a term ($\Phi_q\sim O((\Delta/\pi)\ln D)$ to Φ, where D is the cutoff. There is also a large, cutoff independent imaginary contribution to Φ, coming from the charge fluctuations occurring on energy scales comparable with the charge-fluctuation scale E_q. In practice, even if we use a finite cutoff D, both terms are large and have to be canceled, by absorbing them into a redefinition of the invarient f-level E_f^* and the f-electron wave-function renormalization constant.

To carry out this procedure, we write the f-electron and boson parts of the Lagrangian as

$$\mathscr{L}(\tau)=\bar{f}_m(\tau)\partial f_m(\tau)+\bar{b}(\tau)\partial b(\tau)$$
$$+[i\dot{\theta}(\tau)+\lambda_0+E_f]Q(\tau)$$
$$-E_f\bar{b}(\tau)b(\tau)-[i\dot{\theta}(\tau)+\lambda_0]Q_0\ . \tag{3.115}$$

The third term is an interaction term between $Q(\tau)$ and the fluctuating field $\tilde{\lambda}(\tau)=i\dot{\theta}+\lambda_0+E_f$. Let us consider the f-electron self-energy at $T=0$ and define

$$\Sigma_f=\Sigma_f(0)\ ,$$
$$Z_f^{-1}=1-\left.\frac{\partial\Sigma_f(\omega)}{\partial\omega}\right|_{\omega=0}\ . \tag{3.116}$$

This enables us to define a renormalized f-electron field by $f_m=(Z_f)^{1/2}f'_m$. In terms of the rescaled field, the Lagrangian becomes

$$\mathscr{L}(\tau)=\bar{f}'_m(\tau)\partial f'_m(\tau)+\bar{b}(\tau)\partial b(\tau)+[i\dot{\theta}(\tau)+\tilde{E}_f]\bar{f}'_m(\tau)f'_m(\tau)-E_f\bar{b}(\tau)b(\tau)-[i\dot{\theta}(\tau)\lambda_0]Q_0+\mathscr{L}\mathrm{ct}(\tau)\ , \tag{3.117}$$

where

$$\tilde{E}_f=E_f+\lambda+\Sigma_f \tag{3.118}$$

is the renormalized f-electron energy and

$$\mathscr{L}_{\mathrm{ct}}(\tau)=(Z_f-1)\bar{f}'_m(\tau)\partial f'_m(\tau)-\Sigma_f\bar{f}'_m(\tau)f'_m(\tau)+(Z_f-1)\lambda(\tau)\bar{f}'_m(\tau)f'_m(\tau) \tag{3.119}$$

are the counterterms that will cancel all the unwanted high-energy terms. We shall now drop the primes on the renormalized fields. The first two terms are corrections to the f propagator, whilst the last term is associated with the renormalization of coupling between $\tilde{\lambda}(\tau)$ and the f electron. One of the effects of the fluctuations is to introduce a vertex correction to the coupling between the $\tilde{\lambda}$ field and the f electron given by

$$\Lambda_{\lambda f}(\nu,\omega)=1+\Gamma_{\lambda f}(\nu,\omega)\ . \tag{3.120}$$

Since the charge Q is conserved, a useful Ward identity comes to our aid,

$$-\frac{\partial\Sigma f(0)}{\partial\omega}=\Gamma_{\lambda f}(0,0)\ . \tag{3.121}$$

The quantity $Z_\lambda^{-1}=1+\Gamma_{\lambda f}(0,0)$, defines the vertex renormalization, and because of the above identity $Z_\lambda=Z_f$. This means that the coupling of $\lambda(\tau)$ to the renormalized f electrons is unchanged, and the counterterm $(Z_f-1)\lambda(\tau)f_m^\dagger f_m$ is precisely the term required to cancel vertex corrections $(\Gamma_{\lambda f}Z_f)\lambda(\tau)f_m^\dagger f_m$.

When we proceed to recompute the free energy with the counterterms, the first two terms of $\mathscr{L}_{\mathrm{ct}}$ introduce the interaction

$$[-i\nu_n\Sigma'_f(0)-\Sigma_f(0)]f_m^\dagger(i\nu_n)f_m(i\nu_n) \tag{3.122}$$

to the f-electron lines, and when we insert these into the saddle-point equations, it is equivalent to replacing ξ by $\xi-\xi\Sigma'_f-\Sigma_f$ to the Fermionic part of the saddle-point equation. Finally, we note from (3.118) that $\lambda=\tilde{E}_f-E_f-\Sigma_0$, so we can put $\lambda+i\Delta(\tilde{r}^2-q_0)\equiv\xi-(E_f^{**}+i\Delta q_0)$, where

$$E_f^{**}=E_f^{*}+\Sigma_f\ , \tag{3.123}$$

leading to the renormalized saddle-point equation

$$\xi-E_{fc}^{**}+\frac{\Delta}{\pi}\left[\tilde{\psi}(\xi)-\ln\frac{\Delta\beta}{2\pi^2 i}\right]+\frac{\Delta}{N\pi}\tilde{\psi}'(\xi)[\Phi(\xi,T)-\Sigma_f-\xi\Sigma'_f]=0\ , \tag{3.124}$$

where $E_{fc}^{**}=E_f^{**}+i\Delta q_0$.

At this point it is unnecessary to laboriously compute Σ_f and Σ'_f, for all we require are their dominate high-energy parts. We can extract these contributions by requiring that at $T=0$,

$$\Phi(\xi,T=0)-\xi\Sigma'_f-\Sigma_f=0\ . \tag{3.125}$$

Since both Σ'_f and Σ_f are real, this implies

$$\Sigma'_f=\mathrm{Im}\Phi_{T=0}/\tilde{\Delta}\ ,\qquad \Sigma_f=\mathrm{Re}\Phi_{T=0}-(\tilde{E}_f/\tilde{\Delta})\mathrm{Im}\Phi_{T=0}\ . \tag{3.126}$$

The subtraction terms so defined do not precisely correspond to the definitions (3.115), but contain small cutoff independent corrections that slightly redefine the renormalization procedure.

To leading order in $O(1/N)$, the shift in the saddle point is then

$$\delta\xi=\xi-\xi_{\mathrm{MFT}}=-\frac{\Delta}{N\pi}\left[\frac{\tilde{\psi}'(\xi)}{1+(\Delta/\pi)\tilde{\psi}'(\xi)}\right][\Phi(\xi,T)-\Sigma_f-\xi\Sigma'_f]\ . \tag{3.127}$$

If we look at the cutoff dependence of E_f^{**} we see that it can be written as

$$E_f^{**}=E_f+\frac{\Delta}{\pi}\left[1-\frac{1}{N}\right]\ln\left[\frac{D}{g(\xi)}\right]\ , \tag{3.128}$$

where $g(\xi)$ is a cutoff independent function of ξ. We recognize this as the Haldane invariant f-level[28,29] position, expressed to order $O(1/N)^2$. The shift in the saddle-point variable ξ can be thought of as the inclusion of a counterterm to the mean-field Hamiltonian that cancels the logarithmic divergences of the f-electron self-energy.

We are now in a position to return to (3.112) and compute the $O(1/N)$ corrections to the thermodynamics. Let us first compute the f occupation by taking the derivative of the unrenormalized free energy with respect to E_f, then replacing ξ by $\xi-\xi\Sigma'_f-\Sigma_F$ to renormalize the final expression. This gives

$$\frac{n_f}{N}=\frac{\partial\,\mathrm{Im}\Omega_c}{\partial E_f}=q-\mathrm{Im}\frac{\xi}{\Delta}\ . \tag{3.129}$$

Let us briefly examine the change in the valence resulting from the fluctuations, in the Kondo limit ($|\xi|\ll\Delta$), at $T=0$, for which

$$\delta n_f=-\left[\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\mathrm{sgn}(\nu)\mathrm{Im}\left[\frac{\nu\mathscr{L}^{-1}(\nu)}{\nu+\xi}\right]-\Sigma'_f\tilde{r}_0^2\right]\ . \tag{3.130}$$

The high-frequency parts in the integral are identical to those appearing in the mean-squared radial fluctuations $\langle \delta\tilde{r}^2 \rangle = -\beta^{-1}\Sigma_n R_{rr}(i\nu_n)$, so we can identify this term as coming from the high-frequency fluctuations about the mean-field theory, which tend to reduce the valence. The second term in (3.130) is the adjustment coming from our renormalization procedure, which adjusts the definition of the quasiparticle, so that at $T=0$, the renormalized f occupation is still equal to $\delta(\mu)/\pi = \tan^{-1}\tilde{\Delta}/\tilde{E}_f$ per channel, satisfying the Friedel sum rule.

In the presence of a field, we must replace $\tilde{\psi}(\xi+\nu)$ in $\mathscr{L}(\nu)$ by $1/N\Sigma_m \tilde{\psi}(\xi_m+\nu)$ where $\xi_m = \xi - g\mu_B mB$. To leading order in B^2

$$1/N\Sigma_m \tilde{\psi}(\xi_m+\nu) = \tilde{\psi}(\xi+\nu) + \tfrac{1}{3}(g\mu_B)^2 j(j+1)B^2\tilde{\psi}'(\xi+\nu) ,$$

the magnetic susceptibility can be determined by differentiating Ω_c with respect to B^2. Expressing

$$\frac{-\partial^2\Omega}{\partial B^2} = \chi_s = \tfrac{1}{3}j(j+1)(2j+1)\tilde{\chi}_s$$

then gives (after making the replacement $\xi \to \Sigma_f + \xi\Sigma_f'$)

$$\tilde{\chi}_s(T) = \tilde{\chi}_s^{\rm MF}(T) = \frac{1}{N}{\rm Im}[\tilde{\chi}_s^{\rm fluc}(T)] ,$$
$$\tilde{\chi}_s^{\rm fluc}(T) = \frac{\Delta}{\pi}\left[\int_{-\infty}^{\infty}\frac{d\nu}{\pi}[n(\nu)+\tfrac{1}{2}]\frac{\tilde{\psi}''(\xi+\nu)-\tilde{\psi}''(\xi)}{\mathscr{L}(\nu)} - \tilde{\psi}''(\xi)(\Sigma_f+\xi\Sigma_f')\right] . \tag{3.131}$$

At $T=0$,

$$\chi_s^{\rm fluc}(0) = -\frac{\Delta}{\pi}{\rm Im}\left[\int_{-\infty}^{\infty}\frac{d\nu}{\pi}[n(\nu)+\tfrac{1}{2}]\frac{1/(\xi+\nu)^2 - 1/\xi^2}{\mathscr{L}(\nu)} - \frac{1}{\xi^2}(\Sigma_f+\xi\Sigma_f')\right] , \tag{3.132}$$

and $\chi_s^{\rm MF} = -{\rm Im}[1/(\pi\xi)]$ as before. The entropy is given by

$$\frac{S}{N} = -\frac{\partial\,{\rm Im}\Omega_c}{\partial T} = \frac{S^{\rm MF}}{N} - \frac{1}{N}{\rm Im}\left[\int_{-\infty}^{\infty}\frac{d\nu\nu\beta^2}{\pi}n(\nu)[1+n(\nu)]\ln\mathscr{L}(\nu) + (1-\xi\tilde{\psi}')\beta(\Sigma_f+\xi\Sigma_f') - \frac{\Delta\beta}{\pi}\left[\int_{-\infty}^{\infty}\frac{d\nu}{\pi}[n(\nu)+\tfrac{1}{2}]\frac{(\xi+\nu)\tilde{\psi}'(\xi+\nu)-\xi\tilde{\psi}'(\xi)}{\mathscr{L}(\nu)} - \tilde{\psi}'(\xi)\Sigma^0\right]\right] . \tag{3.133}$$

We can now extract the linear coefficient γ of the specific heat at $T=0$, either by taking the $T\to 0$ limit of dS/dT, or by computing $-2\,\partial\Omega/\partial(T^2)$ at $T=0$ directly. Either method gives $\gamma = \frac{1}{3}N(k_B\pi)^2\tilde{\gamma}$ with

$$\tilde{\gamma} = \left[\tilde{\chi}_s^{\rm MF}(0) + \frac{1}{N}\tilde{\chi}_s^{\rm fluc}(0)\right] - \frac{1}{\pi N}\lim_{\nu\to 0}\frac{\partial}{\partial\nu}[{\rm Im}\ln\mathscr{L}(\nu)] , \tag{3.134}$$

where we have identified the first two terms with corresponding terms in (3.105), and the last term comes from the Bose function in the fluctuation correction to Ω_c. Directly calculating this term we find that

$$\tilde{\gamma} = \tilde{\chi}_s(0) - \frac{1}{N\pi}{\rm Im}\left[\frac{1}{\xi}\left[1 - \frac{1}{1+\Delta/\pi\xi}\right]\right] . \tag{3.135}$$

Using (3.65), to leading order in $O(1/N)$, the second term in (3.135) is equal to the difference between the linear specific-heat coefficient and the charge susceptibility $(1/N)[\tilde{\gamma} - \tilde{\chi}_c(0)]$ in the ground state, so combining (3.134) and (3.132) we find that

$$\tilde{\gamma} = \left[\frac{N}{N-1}\right]\tilde{\chi}_s + \frac{\tilde{\chi}_c}{N} + O(1/N^2) , \tag{3.136}$$

which is the Yamada-Yosida thermodynamic identity for the generalized Anderson model. In the limit that charge fluctuations vanish, this leads to the Wilson ratio $\tilde{\chi}_s/\tilde{\gamma} = N/(N-1)$.

In our treatment we have carried out a very elementary regularization procedure. Read and Newns note that it is possible to carry out a more complete renormalization process where wave-function renormalization counterterms are included into the Lagrangian. In such a treatment, the fluctuation term $\tilde{\chi}^{\rm fluc}$ becomes absorbed into the renormalizations. We have avoided this approach here because it is cumbersome to compute the quasiparticle self-energies.

We have numerically computed the leading $1/N$ corrections and plotted an example of the thermodynamic functions in Fig. 12. We find that they are not singular, even as we approach the mean-field phase transition.

To extend the calculations to high temperatures we have found that there are serious technical difficulties at the crossover. The second-order phase transition present in mean-field theory implies a discontinuity in

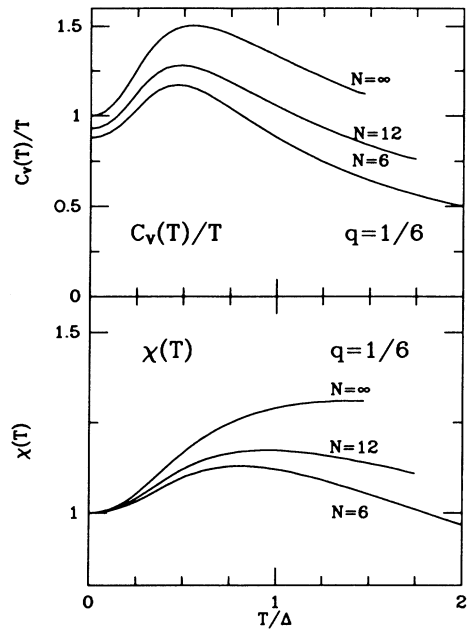

FIG. 12. Leading $1/N$ corrections to the susceptibility and specific heat for the case $Q/N=\frac{1}{6}$, in the Kondo limit. The mean-field parameters have been adjusted so that $\tilde{\chi}$ is constant and the curves are normalized with respect to their value at $T=0$, $N=\infty$. Note how the Wilson ratio rises as the spin degeneracy increases.

$C_V/T=-d^2\Omega/dT^2$ at the crossover, and clearly the $1/N$ expansion is singular at the crossover in the large-N limit. This is a common drawback of large N expansions, and it comes about because one has taken the macroscopic limit of the system, leading to an arbitrarily sharp crossover.[44] We can attempt to analytically extend our results through the crossover by using the effective action evaluated with the Gaussian fluctuations included, and evaluate the saddle-point condition (3.124) self-consistently. However, the results will not contain the discontinuity as $N\rightarrow\infty$.

It is possible to carry out an analysis around the weak coupling saddle point at $b=0$, using the Cartesian Bose coordinates. Such an analysis shows that the $1/N$ corrections are *divergent* at the crossover, in contrast to the strong coupling side, where the expansion is not singular but is probably missing nonperturbative terms. Similar behavior has been well documented in simple matrix models,[44] where the corrections to mean field have different forms in weak and strong coupling.

It seems very likely that as in many other crossover phenomenon, (such as the crossover to high temperatures in one-dimensional spin chains and the metal-insulator transition), there are terms which affect the crossover region that cannot be expanded perturbatively. In our strong coupling treatment these come from the need to restrict radial fluctuations to being positive, and initial analysis of the corrections arising from the "hard-core repulsion" that this adds to the effective potential indicate that there are new terms of the form e^{-N} entering into the effective potential. These terms are not important until one reaches the crossover regime where the effective potential for radial fluctuations becomes very flat.

In conclusion to this section, whilst we are able to compute the leading corrections to the saddle point in the strongly coupled Fermi-liquid regime of the model, the crossover to weak coupling cannot be dealt with using just the Gaussian fluctuations. This remains a challenging problem for future work.

IV. TWO IMPURITIES

A. Nonlocal charge and spin fluctuations

As our second example we shall calculate the nonlocal correlations and interactions in the two impurity model. In our model the presence of nonlocal fluctuations is signaled by two independent nondegenerate modes of oscillation in the Bose field which arise from spin and charge fluctuations which are either symmetric or antisymmetric with respect to reflection in the plane separating the two ions. Since there are now two conserved charges, both modes contain a low-energy zero mode, which means that intersite and intrasite couplings between the electrons in the Cartesian gauge contain a strong coupling divergence. Had we attempted to treat the two-impurity model in a renormalization-group picture, we would expect to find two corresponding relevant operators with a strong coupling fixed point at low temperatures.

We shall deal with the zero modes exactly as before using the radial gauge of Newns and Read. The analysis carried out explicitly in Sec. III B can be repeated for an arbitrary number of mixed valence ions by considering the Bose-field integrations for each site separately. In the two-impurity model this means integrating over the amplitude and phase velocity fluctuations at two sites, so the full partition function becomes

$$Z_{\rm MV}=\int \mathscr{D}[\bar{\psi},\psi]\mathscr{D}[r_1,\dot{\theta}_1]\mathscr{D}[r_2,\dot{\theta}_2]e^{-\int_0^\beta \mathscr{L}(\tau)d\tau}\ , \tag{4.1}$$

where $\mathscr{L}(\tau)$ now contains an interaction term for each site

$$\mathscr{L}_{\rm int}(\tau)=\sum_{j=1,2}\left\{ i\dot{\theta}_j(\tau)Q(\mathbf{R}_j,\tau) + \frac{V(k)}{\sqrt{N}}\sum_{m,k}[c^\dagger_{\mathbf{k}m}f_m(\mathbf{R}_j)e^{-i\mathbf{k}\cdot\mathbf{R}_j} + \text{H.c.}]r_j(\tau)\right\}. \tag{4.2}$$

Now in our mean-field solution of Sec. II E the static value of $r/\sqrt{N}=r_0$ is the same at both sites. When we expand the Lagrangian in small fluctuations it is convenient to define antisymmetric and symmetric fluctuation modes

$$\begin{aligned}\delta r^{\pm}(\tau)&=\frac{1}{\sqrt{2}}[\delta\tilde{r}_1(\tau)\pm\delta\tilde{r}_2(\tau)]\ ,\\ \dot{\theta}^{\pm}(\tau)&=\frac{1}{\sqrt{2}}[\dot{\theta}_1(\tau)\pm\dot{\theta}_2(\tau)]\ ,\end{aligned} \tag{4.3}$$

in terms of which the interaction Lagrangian takes the form

$$\mathscr{L}_{\rm int}(\tau)=\frac{1}{\sqrt{2}}\left[i\dot{\theta}^{+}\sum_{p}n_f^p+\delta\mathbf{r}^{+}(\tau)\sum_{p,m,k}V^p(k)[c_{km}^{(p)+}f_m^{(p)}+\text{H.c.}]\right]$$
$$+\frac{1}{\sqrt{2}}\left[i\dot{\theta}^{-}\sum_{p,m}f_m^{+(p)}f_m^{(-p)}+\delta\tilde{r}^{-}(\tau)\sum_{p,m,k}V^p(k)[c_{km}^{+(p)}f_m^{(-p)}+\text{H.c.}]\right], \tag{4.4}$$

showing that the total parity is conserved: even-parity fluctuations conserve the parity of electrons they interact with; odd-parity fluctuations flip the parity of the states they interact with. This is the two-impurity version of lattice momentum conservation. In the corresponding Feynman diagrams, we make sure that parity is always conserved at interaction vertices.

When we expand the effective free-energy functional about the mean-field value, parity conservation ensures that it is diagonal in the even- and odd-parity Gaussian fluctuations

$$\beta\Omega_{\rm eff}=\beta\Omega_0+\frac{1}{2}\sum_{p=\pm1}\int d\tau_1 d\tau_2\mathbf{r}^p(\tau_2)\cdot\Gamma^p(\tau_2-\tau_1)\cdot\mathbf{r}^p(\tau_1) \tag{4.5}$$

where

$$\Omega_0=\sum_m\sum_{p=\pm1}\int\frac{f(\omega)}{\pi}\delta_m^p(\omega),\quad \delta_m^p(\omega)=\tan^{-1}\left[\frac{\tilde{\Delta}^p}{\tilde{E}_{fm}-\omega}\right] \tag{4.6}$$

is the mean-field free energy, $\bar{\mathbf{r}}^p=(\delta\tilde{r}^p,i\tilde{r}_0\dot{\theta}^p)$, and $\Gamma^p(\tau)$ has the same form as before,

$$\Gamma^p=\Gamma^{(0)}+\Pi^p\ . \tag{4.7}$$

The RPA polarization graphs entering into π^p are similar to the one-impurity model, excepting that two values of parity must be summed over in the Fermion loops. For Π^+ the internal electron lines have the same parity, while for Π^- the internal electron lines have opposite parity (Fig. 13).

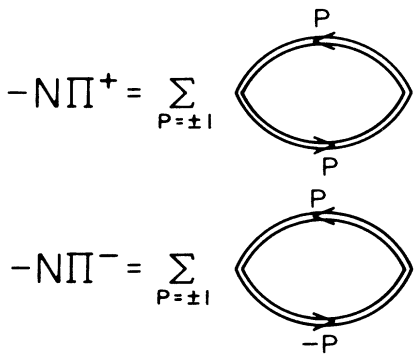

FIG. 13. Antisymmetric (−) and symmetric (+) RPA self-energies for the two-impurity model, showing just the parities of the fermion propagators. (See Fig. 5 for the coupling between the propagators and the fluctuations.)

The calculation of these polarization diagrams is repeated exactly as for the one-impurity model assuming a large bandwidth cutoff, and we can actually derive analytic results provided we make the near field assumption discussed in II E assuming that $T_K\ll v_F\hbar/\tilde{\Delta}$, enabling us to treat the two channels as nondegenerate Lorentzian resonances. The simple symmetries apparent in the one impurity expressions are now lost and we find the following results for the symmetric RPA diagrams

$$\Gamma_{rr}^{+}=\sum_{p=\pm1}\text{Re}\left[\frac{1}{g^p(i\nu_n)}\mathscr{L}^p(i\nu_n)\right]+\tilde{t}^2\Gamma_{\dot{\theta}\dot{\theta}}^{+},$$
$$\Gamma_{r\dot{\theta}}^{+}(i\nu_n)=\sum_{p=\pm1}\frac{1}{\nu_n}\text{Im}[\mathscr{L}^p(i\nu_n)+i\nu_n]$$
$$-\text{Re}\left[\frac{p\tilde{t}g^p(i\nu_n)}{\nu_n^2}\mathscr{L}^p(i\nu_n)\right], \tag{4.8}$$
$$\Gamma_{\dot{\theta}\dot{\theta}}^{+}(i\nu_n)=\sum_{p=\pm1}-\text{Re}\left[\frac{g^p(i\nu_n)}{\nu_n^2}\mathscr{L}^p(i\nu_n)\right],$$

where

$$\mathscr{L}^p(i\nu_n)=\frac{\Delta^p-ip\cdot t}{\pi}[\tilde{\psi}(\xi^p+i\nu_n)-\tilde{\psi}(\xi^p)],$$
$$g^p(i\nu_n)=\frac{\nu_n}{\nu_n+2\tilde{\Delta}^p}, \tag{4.9}$$

with $\xi^p=\tilde{E}_f+p\tilde{t}(R)+i\tilde{\Delta}^p$, $\tilde{\Delta}^p=\Delta p\tilde{r}_0^2$, $\tilde{t}(R)=\tilde{r}_0^2t(R)$, and $\Delta^p=\Delta[1+pj_0(k_FR)]$ as before. For the antisymmetric RPA diagrams we find

$$\Gamma_{rr}^{-}(i\nu_n)=\sum_{p=\pm1}\text{Re}\left[\frac{1}{h^p(i\nu_n)}[\mathscr{L}_1^p(i\nu_n)-ps\mathscr{L}_2^p(i\nu_n)]\right],$$
$$\Gamma_{r\dot{\theta}}^{-}(i\nu_n)=\sum_{p=\pm1}\frac{1}{\nu_n}\text{Im}[\mathscr{L}_1^p(i\nu_n)-ps\mathscr{L}_2^p(i\nu_n)+i\nu_n], \tag{4.10}$$
$$\Gamma_{\dot{\theta}\dot{\theta}}^{-}(i\nu_n)=-\sum_{p=\pm1}\frac{1}{2\tilde{\Delta}\nu_n}\text{Re}[\mathscr{L}_1^p(i\nu_n)-\mathscr{L}_2^p(i\nu_n)],$$

where

$$\mathscr{L}_1^p=\frac{i\nu_n}{i\nu_n+(\xi^p-\xi^{-p})}\frac{\Delta}{\pi}[\psi(\xi^p+i\nu_n)-\psi(\xi^{-p})],$$
$$\mathscr{L}_2^p=\frac{i\nu_n}{i\nu_n+(\xi^p-\xi^{*-p})}\frac{\Delta}{\pi}[\psi(\xi^p+i\nu_n)-\psi(\xi^{-p})^*], \tag{4.11}$$
$$h^p(i\nu_n)=\frac{i\nu_n}{i\nu_n+(\xi^p-\xi^{-p})+2i\tilde{\Delta}},$$

with $s=j_0(k_FR)$, $\tilde{\Delta}=\Delta r_0^2$, and $\gamma=t/\Delta=\tilde{t}/\tilde{\Delta}$ as before.

Corresponding to the Γ^p are the symmetric and antisymmetric Bose propagators, given by

$$\begin{aligned}\langle T\bar{\mathbf{r}}^p(i\nu_n)\bar{\mathbf{r}}^p(-i\nu_n)\rangle &= \frac{1}{N}R^p(i\nu_n) \\ &= \frac{1}{N}[\Gamma^p(i\nu_n)]^{-1} \\ &= \frac{1}{N}\frac{1}{[\Gamma_{rr}\Gamma_{\dot\theta\dot\theta}-(\Gamma_{\dot\theta r})^2]}\begin{bmatrix}\Gamma_{\dot\theta\dot\theta} & -\Gamma_{r\dot\theta}\\ -\Gamma_{r\dot\theta} & \Gamma_{rr}\end{bmatrix}. \end{aligned} \tag{4.12}$$

Lavagna[30] has suggested the interesting possibility of an instability in the antisymmetric fluctuations at a lower temperature than the mean-field instability in the symmetric fluctuations, but restricts her analysis to the case when $\tilde{r}_0=0$. To check this hypothesis, one needs to take the mean field $\mathbf{r}_0$ of the symmetric fluctuations into account. The appearance of such an instability would be signaled by a singularity in the antisymmetric propagators we have derived above. However, these propagators are not singular provided $\tilde{r}_0\neq 0$. In other words the development of a symmetric mean field rules out any subsequent instability of the antisymmetric fluctuations.

We will relate these functions to the spin and charge susceptibilities. Note that intrasite and intersite correlations are determined by

$$\begin{aligned}\langle \bar{\mathbf{r}}_1(i\nu_n)\bar{\mathbf{r}}_1(-i\nu_n)\rangle &= \tfrac{1}{2}[R^+(i\nu_n)+R^-(i\nu_n)], \\ \langle \bar{\mathbf{r}}_1(i\nu_n)\bar{\mathbf{r}}_2(-i\nu_n)\rangle &= \tfrac{1}{2}[R^+(i\nu_n)-R^-(i\nu_n)].\end{aligned} \tag{4.13}$$

B. Charge and spin susceptibilities

Since the Gaussian effective free energy is diagonal in the even and odd fluctuations, the derivations of Sec. III D can be repeated for each boson mode. We can write down the even- and odd-parity susceptibilities directly, as

$$\begin{aligned}\frac{\chi_c^p}{N^2}(\tau) &= \langle T\delta\tilde{n}^p_f(\tau)\delta\tilde{n}^p_f(0)\rangle = 4\tilde{r}_0^2\langle T\delta\tilde{r}^p(\tau)\delta\tilde{r}^p(0)\rangle, \\ \chi_s(\tau) &= \langle TM_z^p(\tau)M_z^p(0)\rangle = \sum_m m^2\frac{1}{N}\frac{\delta^2\Omega_{\rm eff}\beta}{N\delta\dot\theta p(\tau)\delta\dot\theta(0)} \\ &= \sum_m m^2[-\tilde{r}_0^2\Pi^p_{\dot\theta\dot\theta}(\tau)],\end{aligned} \tag{4.14}$$

where

$$\begin{aligned}\delta\tilde{n}^p &= \frac{1}{N}\sum_m f_m^{p+}f_m^p - \frac{\langle n^p\rangle}{N}, \\ M_z^p &= \sum_m m f_m^{p+}f_m^p .\end{aligned}$$

We can directly calculate the static spin susceptibilities by taking the zero-frequency limits of $\tilde{\chi}^p(i\nu_n)=-\tilde{r}_0^2\Pi^p_{\dot\theta\dot\theta}(i\nu_n)$, whereupon we find (for $T=0$)

$$\begin{aligned}\tilde{\chi}^-(0) &= \mathrm{Re}\frac{1}{\pi(\tilde{\Delta}s-i\tilde{t})}\ln\frac{\xi^+}{\xi^-}, \\ \tilde{\chi}^+(0) &= \frac{1}{2\pi}\sum_{p=\pm}\frac{\tilde{\Delta}^p}{|\xi^p|^2}.\end{aligned} \tag{4.15}$$

In the limit of large separations $\tilde{\Delta}^+$ and $\tilde{\Delta}^-\to\tilde{\Delta}$, while $\tilde{t}(R)\to 0$ so that

$$\tilde{\chi}^{\pm}\underset{(R\to\infty)}{\to}\frac{1}{\pi}\left[\frac{\tilde{\Delta}}{\tilde{\Delta}^2+\tilde{E}_f^2}\right] \tag{4.16}$$

which is exactly the single impurity result. We can calculate the intersite spin susceptibility as

$$\tilde{\chi}_{12}=\frac{1}{2}\left[\frac{1}{2\pi}\sum\frac{\tilde{\Delta}^p}{|\xi^p|^2}-\mathrm{Re}\frac{1}{\pi[\tilde{\Delta}s-i\tilde{t}(R)]}\ln\frac{\xi^+}{\xi^-}\right]. \tag{4.17}$$

There are two competing terms in this susceptibility of opposite sign.

The size and magnitude of the intersite hopping parameter $\tilde{t}$ dramatically affects the size and sign of the intersite spin correlations. If we set this parameter to zero, then the intersite spin correlations oscillate without changing sign as the separation of the ions is changed. If we allow a more realistic variation of $t(R)$ with separation, such as that generated by a parabolic band, then oscillatory intersite spin correlations reminiscent of the RKKY interaction are exhibited.

For small separations of the ions, the spin correlations are dramatically dependent on the degree of filling of the f states. As $R\to 0$, the antisymmetric quasiparticle resonance width tends to zero, whilst the splitting of the resonances $\tilde{r}_0^2t(R)$ tends to a constant. Depending on the size of $t(0)$, and the filling factor of the f states $\tilde{n}_f=[n_f(R_1)+n_f(R_2)]/2(2j+1)$, the antisymmetric resonance is either partially full, leading to an unquenched moment at $R=0$, or it is completely full or empty, leading to a quenched groundstate at $R=0$. The latter condition occurs if $\tilde{n}_f\notin(f,f+\frac{1}{2})$, where $f=1/\pi\tan^{-1}\{\Delta/-t(R=0)]\}$, and for small R we shall call this occupation regime the "strongly quenched regime". If the filling is between f and $f+\frac{1}{2}$, the antisymmetric resonance is partially filled, in which case the f level becomes pinned to the Fermi level and the susceptibilities diverge as $R\to 0$. Direct calculation shows that in the limit $R\to 0$

$$\begin{aligned}\chi^+ &= O\left[\frac{1}{R}\right], \\ \chi^- &= O\left[\ln\left[\frac{1}{R}\right]\right]\end{aligned} \tag{4.18}$$

for small R. We shall call this regime the "weakly quenched regime".

We have solved the saddle-point equations (2.101) numerically, and plotted $\tilde{\chi}_+$ and $\tilde{\chi}_-$ in Fig. 14. The position of the nodes where $\chi_{12}=\frac{1}{2}(\chi^+-\chi^-)$ vanishes is found to depend on the band symmetry k_D/k_F. One of the most interesting features to emerge is the appearance

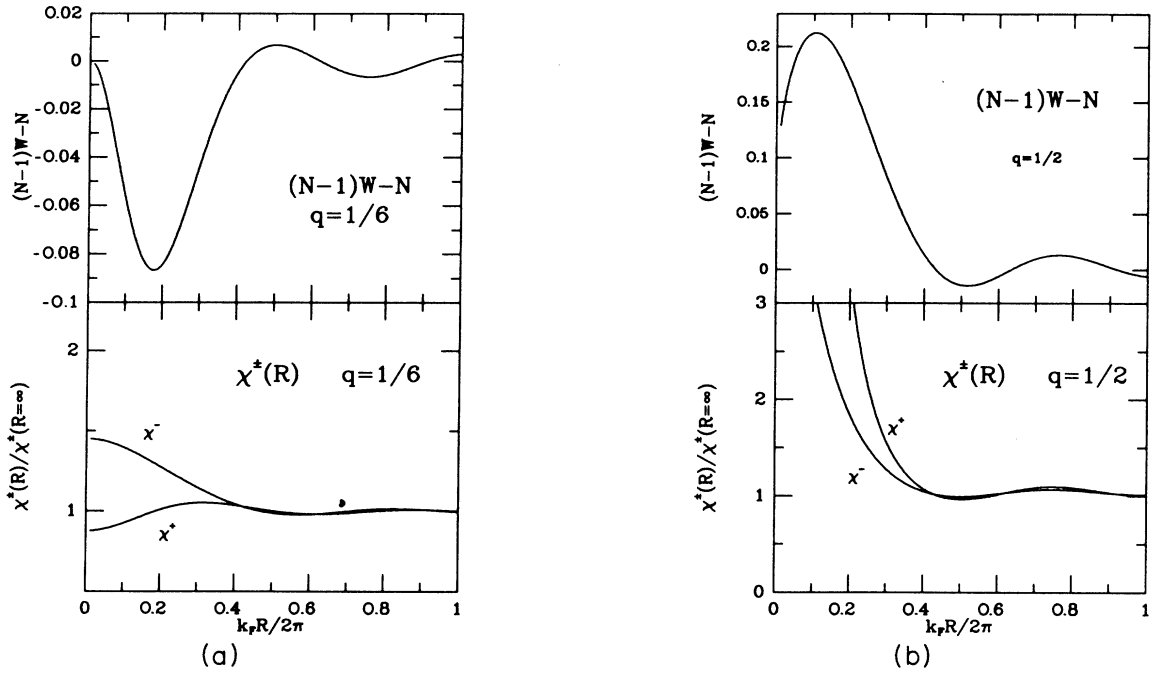

FIG. 14. (a) Showing for $q=\frac{1}{6}$ and $k_D/k_F=1.196$ (i) the deviation of the Wilson Ratio $W=\tilde{\chi}/\tilde{\gamma}$ from its one impurity value $N/(N-1)$ in the Kondo limit and (ii) the symmetric $\tilde{\chi}^{+}(R)$ and antisymmetric $\tilde{\chi}^{-}(R)$ susceptibilities as a function of R in the Kondo limit. The ground state is fully quenched for all R, and the correlations are intrinsically antiferromagnetic, with a reduced Wilson ratio. (b) Showing for $q=\frac{1}{2}$ and $k_D/k_F=1.196$ (i) the deviation of the Wilson Ratio $W=\tilde{\chi}/\tilde{\gamma}$ from its one-impurity value $N/(N-1)$ in the Kondo limit and (ii) the symmetric $\tilde{\chi}^{+}(R)$ and antisymmetric $\tilde{\chi}^{-}(R)$ susceptibilities as a function of R in the Kondo limit. Here the ground-state f moments are weakly quenched at small separations and the correlations are ferromagnetic, with an increased Wilson ratio.

of a ferromagnetic intersite spin correlation in the weakly quenched regime. In the strongly quenched regime the intersite susceptibility becomes antiferromagnetic. This is reminiscent of the strong dependence of intersite spin correlations on filling factor and intersite hopping in the Alexander-Anderson model for two magnetic impurities,[45–47] although at small R we see that the intersite spin correlation is ferromagnetic at half filling, instead of antiferromagnetic in the case of direct f-f hopping.

In the following section we shall see how this feature is reflected in the interactions.

Extrapolating our results to finite degeneracy, we expect to see similar dramatic effects upon changing the filling factor. Thus, if we take $n_f=1$ at each site, then changing the spin degeneracy from two to four should change the sign of the intersite spin correlations at short distances.

Figure 15 shows the dynamical spin susceptibilities for the corresponding cases, clearly displaying that the even and odd modes only split their degeneracy at low energies comparable with $\tilde{\Delta}$, where there is considerable intersite hopping of the heavy quasiparticles. By contrast, since most of the charge fluctuations occur at energies much greater than the spin-fluctuation scale, the symmetric and antisymmetric charge fluctuations are essentially degenerate in the Kondo limit so that charge fluctuations are local.

Finally, we note that as in the one-impurity case we find, on repeating the analysis of Sec. III D that the even and odd Gaussian fluctuations in q are identically zero. Rather than presenting a specific analysis, we refer the reader to the general proof given in Appendix C that q

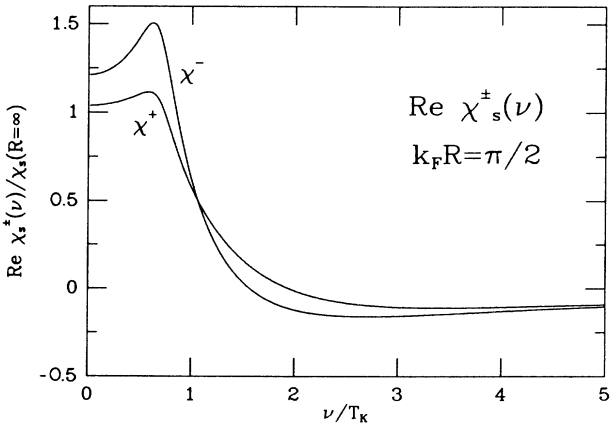

FIG. 15. Showing the antisymmetric and symmetric dynamical spin susceptibilities for the case $q=\frac{1}{6}$ and $k_FR=\pi/2$. The antisymmetric susceptibility is largest at low frequency, leading to antiferromagnetic spin correlations between sites.

fluctuations are conserved in the Gaussian fluctuation for an arbitrary number of magnetic scatterers.

C. Interactions in the two-impurity model

In this section we examine the nature of the electronic interactions in the large-N limit of the generalized Anderson model, discussing the high- and low-energy behavior.

1. Influence of zero modes on the RKKY interaction

Using the controlled results for fluctuations in the radial gauge, the fluctuations in the Cartesian gauge can be derived. This enables us to make contact with the weak coupling perturbative picture of the two-impurity model. As in the two-impurity model, the presence of zero modes drives the interactions to strong coupling at low frequencies, and from the low-frequency spectrum of the phase fluctuations, we can determine the scaling of the interactions in strong coupling.

The fluctuations of the slave boson field lead to an effective on-site interaction which has the same form as in the one-impurity model,

$$\beta\hat{H}_i=-\frac{1}{N}\int_0^\beta d\tau\, d\tau'\sigma_i^\dagger(\tau)J(\tau-\tau')\sigma_i(\tau')\ , \tag{4.19}$$

where $\sigma_i=\Sigma_{\mathbf{k},m}f_m c_{\mathbf{k}m}e^{i\mathbf{k}\cdot\mathbf{R}_j}$ as before, and $J(\tau)=V^2\langle Tb_i(\tau)b_i^\dagger\rangle$. Of particular interest however, is the spin-dependent intersite interaction between the f electrons that is generated by the fluctuations. This has the form

$$\beta H_{12}=\frac{V^4}{N_2}\int_0^\beta\prod_{j=1}^4 d\tau_j\Gamma_{12}(\tau_1,\tau_1';\tau_2,\tau_2')[f_m(1,\tau_1)f_{m'}(2,\tau_2)f_{m'}^\dagger(1,\tau_1')f_m^\dagger(2,\tau_2')]\ , \tag{4.20}$$

where

$$\Gamma_{12}(\tau_1,\tau_1';\tau_2,\tau_2')=\langle T[d_m(\mathbf{R}_1,\tau_1')d_{m'}(\mathbf{R}_2,\tau_2')d_{m'}^\dagger(\mathbf{R}_1,\tau_1)d_m^\dagger(\mathbf{R}_2,\tau_2)]\rangle\quad(m\neq m') \tag{4.21}$$

and the shorthand

$$d_m^\dagger(\mathbf{R}_j,\tau)=\Sigma_{\mathbf{k}}c_{\mathbf{k}m}^\dagger(\tau)b^\dagger(\mathbf{R}_j,\tau)e^{i\mathbf{k}\cdot\mathbf{R}_j}$$

is used. In (4.21) $m\neq m'$ to exclude the spin-independent part of the intersite interaction. At frequencies below the charge fluctuation scale E_q, this is an interaction between the spin degrees of freedom at the neighboring sites, and will be referred to as an "RKKY" interaction.

At high energies the on-site interaction becomes identical to the one-impurity problem, discussed in Sec. III F. However, at low energies the zero mode is modified by intersite coherence. As before, we have

$$\lim_{\tau\to\infty}\langle b_j(\tau)b_j^\dagger(0)\rangle=r_0^2\langle e^{i[\theta_j(\tau)-\theta_j(0)]}\rangle$$
$$=r_0^2e^{-1/2\langle\delta\theta_j(\tau)^2\rangle} \tag{4.22}$$

in the Gaussian approximation. In the two-impurity problem, there are two zero modes, corresponding to the antisymmetric and symmetric phase fluctuations. A simple extension of the one impurity derivation gives

$$\tfrac{1}{2}\langle\delta\theta_j(\tau)^2\rangle=\frac{1}{N}\left[\frac{\alpha^++\alpha^-}{2}\right]\ln\left[\frac{\tau}{C}\right]\ , \tag{4.23}$$

where

$$\frac{\alpha^P}{N}=\lim_{\nu\to0}\mathrm{Im}\left[\frac{1}{\nu\tilde{r}_0^2\pi}R^P_{\theta\theta}(\nu)\right]\ . \tag{4.24}$$

Infrared divergences are also present in the intersite interaction, as we shall now show. The singular behavior in Γ_{12} arises from the changes in Q_1 and Q_2, resulting from the bose operators. The conduction electrons do not carry the charges Q_i, so that self-energy and vertex insertions to the conduction-electron part of Γ_{12} will not modify the infrared singularities of the full vertex. This enables us to approximate Γ_{12} as a product of a boson and a conduction electron vertex $\Gamma_{12}=\Gamma_{12}^{\text{fermion}}\Gamma_{12}^{\text{boson}}$, where the singular behavior at low frequencies is contained in the Bose part. This then gives an approximation containing the important amomalous singular properties at low energies, and the leading $O(1/N^2)$ contribution to the perturbative RKKY interaction at high energies. In this approximation we shall include no self-energy or vertex corrections to the conduction-electron lines, (other than the mean-field corrections) so that

$$\Gamma_{12}^{\text{fermion}}=\langle Tc_m(1,\tau_1')c_m^\dagger(2,\tau_2)\rangle_{\text{MF}}$$
$$\times\langle Tc_{m'}(2,\tau_2')c_{m'}^\dagger(1,\tau_1)\rangle_{\text{MF}} \tag{4.25}$$

where the conduction propagators are evaluated in the mean field theory. The boson vertex,

$$\Gamma_{12}^{\text{boson}}=\langle Tb(1,\tau_1')b(2,\tau_2')b^\dagger(2,\tau_2)b^\dagger(1,\tau_1)\rangle \tag{4.26}$$

will now be studied carefully.

At high frequencies and short times, intersite correlations of the boson fluctuations are weak, enabling further factorization

$$\Gamma_{12}^{\text{boson}}=\langle Tb(1,\tau_1')b^\dagger(1,\tau_1)\rangle\langle Tb(2,\tau_2')b^\dagger(2,\tau_2)\rangle\ . \tag{4.27}$$

Provided that the time scales of interest are larger than the characteristic charge fluctuation time $1/E_q$, but much shorter than $1/T_K$, then we can approximate the high-frequency contribution to the Bose propagator by $\langle Tb(\tau)b^\dagger(0)\rangle\sim e^{-E_q\tau}\sim(1/E_q)\delta(\tau)$. The intersite interaction is then approximately

$$\frac{V^4}{N^2}\Gamma_{12}\approx[\delta(\tau_1-\tau_1')\delta(\tau_2-\tau_2')J^2/N^2]$$
$$\times\sum_{\mathbf{k},\mathbf{k}'}G_{\mathbf{k}}(\tau_1-\tau_2)G_{\mathbf{k}'}(\tau_2-\tau_1)e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}}\ , \tag{4.28}$$

with $J=V^2/E_q$. Evaluation of the summation at equal times gives the conventional perturbative RKKY interaction.

At low energies however, we cannot factorize the Bose vertex, and the divergent zero modes dominate the infrared behavior of the interaction, leading to

$$\Gamma_{12}^{\text{boson}} \approx r_0^4 \langle \exp i[\theta_1(\tau_1')+\theta_2(\tau_2')-\theta_1(\tau_1)-\theta_2(\tau_2)] \rangle \ . \quad (4.29)$$

Using the Gaussian fluctuations this function is given by

$$\Gamma_{12}^{\text{boson}} \approx r_0^4 \exp -\tfrac{1}{2} \langle [\theta_1(\tau_1')+\theta_2(\tau_2') -\theta_1(\tau_1)-\theta_2(\tau_2)]^2 \rangle \ . \quad (4.30)$$

Putting $\theta_1=\frac{1}{2}(\theta^+ +\theta^-)$ and $\theta_2=\frac{1}{2}(\theta^+ -\theta^-)$, and expanding the exponent in symmetric and antisymmetric modes then gives

$$\Gamma_{12}^{\text{boson}} \approx r_0^4 \exp -[C^+(\tau_1,\tau_1';\tau_2,\tau_2')+C^-(\tau_1,\tau_1';\tau_2,\tau_2')] \ , \quad (4.31)$$

where

$$C^p(\tau_1,\tau_1';\tau_2,\tau_2')=\tfrac{1}{8}\langle \{\theta^p(\tau_1')-\theta^p(\tau_1') +p[\theta^p(\tau_2')-\theta^p(\tau_2)]\}^2 \rangle \ . \quad (4.32)$$

In the long-time approximation, when τ_1, τ_1', τ_2, and τ_2' are well separated,

$$C^p(\tau_1,\tau_1';\tau_2,\tau_2')=\frac{\alpha^p}{4}\ln\left[|\tau_1'-\tau_1| \ |\tau_2-\tau_2'| \left[\frac{|\tau_1'-\tau_2| \ |\tau_2'-\tau_1|}{|\tau_1-\tau_2| \ |\tau_1'-\tau_2'|} \right]^p \right] . \quad (4.33)$$

Similar Green's functions appear in the x-ray edge solution of Nozières and de Dominicis,[14] and although the techniques employed are quite different, the power-law relaxation appearing here has a similar origin. From (4.31), it follows that

$$\lim_{\tau\to\infty} \langle T b_1(\tau)b_2(\tau)b_1^\dagger(0)b_2^\dagger(0)\rangle \sim (\tau)^{-\alpha^+/N} \ ,$$
$$\lim_{\tau\to\infty} \langle T b_1^\dagger(\tau)b_2(\tau)b_1(0)b_2^\dagger(0)\rangle \sim (\tau)^{-\alpha^-/N} \ . \quad (4.34)$$

The operators $b_1^\dagger b_2^\dagger$ and $b_1^\dagger b_2$ increase $Q^p=\frac{1}{2}(Q_1+pQ_2)$ by one, respectively, and the α^p/N are the corresponding x-ray exponents. In this case, increasing Q^p by one changes the phase shift in both even- and odd-parity channels. For the symmetric exponent, the action of $b_1^\dagger b_2^\dagger$ preserves the reflection symmetry of the state, so we expect Nozières-de Dominicis x-ray-type arguments hold for this case, so that

$$\alpha^+ = \left[\frac{dn_f^+}{dQ^+}\right]^2 + \left[\frac{dn_f^-}{dQ^+}\right]^2 ,$$

a relation which has been confirmed by to hold precisely in numerical calculations of the symmetric fluctuations, but as yet algebraic proof is lacking. For the antisymmetric exponent, the final state no longer has reflection symmetry, and it is unclear whether single impurity Nozières—de Dominicis arguments work in detail.

From the above results, we deduce that there are two independent singularities in the RKKY interaction at low energies:

(i) Electron-electron channel,

$$V_{ee}(\tau,\tau') \sim \frac{\tilde{r}_0^4}{|\tau-\tau'|^{2+\alpha^+/N}} \sum_{m,m'} [f_m^\dagger(1,\tau)f_{m'}^\dagger(2,\tau)f_{m'}(1,\tau')f_m(2,\tau')] \ , \quad (4.35)$$

where the additional power of 2 comes from the intersite electron propagators $\langle c_m(1,\tau)c_m^\dagger(2,0)\rangle$ $1/\tau$, and is a term present in the conventional RKKY interaction. This singularity leads to terms of the form $\nu^{[1+(\alpha^+/N)]}$, upon Fourier transforming, and therefore introduces no strong coupling divergence of the interaction.

(ii) Electron-hole channel,

$$V_{eh}(\tau,\tau') \sim \frac{\tilde{r}_0^4}{|\tau-\tau'|^{\alpha^-/N}} \sum_{m,m'} [f_m^\dagger(2,\tau)f_m(1,\tau)f_{m'}^\dagger(2,\tau')f_{m'}(1,\tau')] \ . \quad (4.36)$$

This term generates a singularity of the form $\nu^{-1+(\alpha^-/N)}$ which scales to strong coupling at low energies. Development of the singularity in this channel is consistent with the treatment of $\langle f_m^\dagger(2,\tau)f_m(1,\tau)\rangle$ as a semiclassical variable describing the development of intersite coherence, and it is this singularity that will lead to an RKKY contribution to the splitting of degeneracy between the symmetric and antisymmetric resonances, as shown in (2.99).

We have calculated the exponents α^p as a function of separation of the two ions, and find that whereas the behavior of the symmetric exponent is similar in the strongly quenched and weakly quenched regimes, the behavior of α^- is markedly different in the two regimes. Figure 16 shows the behavior of these two exponents in the Kondo limit. At large separations, the α^p are degenerate. At small separations $\alpha^+ \to 2$ which is consistent with only the symmetric channel coupling to fluctuations, experiencing a phase shift change of $2\pi/N$ per channel after the operation of $b_1^\dagger b_2^\dagger$. However, $\alpha^- \to 0$ in the strongly quenched regime, whilst $\alpha^- \to \infty$ in the weakly

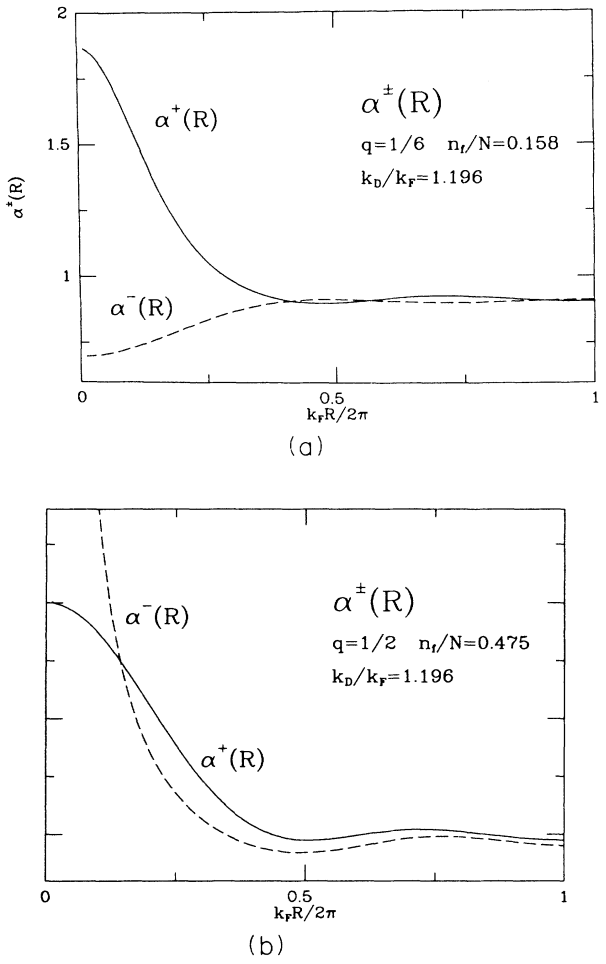

FIG. 16. (a) $\alpha^+(R)$ and $\alpha^-(R)$ for the case $q=\frac{1}{6}$. (b) $\alpha^+(R)$ and $\alpha^-(R)$ for the case $q=\frac{1}{2}$. The divergence of $\alpha^-(R)$ at small separations suggests that the Fermi-liquid picture used here becomes inappropriate for small distances.

quenched regime as $R\to 0$. The largeness of α^- in the weakly quenched regime indicates that antisymmetric correlations die away rapidly with time. This presumably is why the symmetric spin susceptibility is greater than the antisymmetric susceptibility, leading to a ferromagnetic susceptibility in this regime. It also implies that at short distance, the mean-field picture must break down, possibly because the RKKY interaction becomes comparable with the spin-fluctuation temperature.

In our arguments above we have not discussed more general intersite interactions that mix the conduction and f-electron spins. In general, for filling factors away from $\frac{1}{2}$, these terms will also be important, and they are subject to the same infrared effects as the RKKY interaction. It is these additional terms which are responsible for the dependence of the intersite spin correlations on filling factor. We will introduce these additional interactions in the following section.

Recent work by Abrahams and Varma[48] on the two-impurity Kondo model, suggests that the RKKY interaction could scale to strong coupling. This result is partly consistent with the arguments advanced here. There is however an important difference, for the strong coupling divergence derived here does not give rise to any additional logarithms in the weak coupling scaling of the RKKY interaction and it is strictly a strong coupling effect resulting from the interference of the two quenched moments. (In other words, there is no additional crossover temperature.) Nevertheless, it is very likely that in a totally analogous fashion to the one-impurity problem, a resonant-level picture of the two-impurity problem can also be gained from consideration of a strong coupling expansion of an appropriate spin model involving strong intersite spin interactions.

We shall now see how the ground-state spin correlations can be understood in terms of the Fermi-liquid properties.

2. *Fermi-liquid properties*

To calculate the Fermi-liquid properties we return to the radial gauge. The calculation is analogous to Sec. III D. We need to calculate how the mean-field scattering potential is modified when we add a quasiparticle of spin m, parity p to the system. Rather than repeat the mean-field calculations in the presence of an additional quasiparticle, we shall extract this information from the Bose propagators.

The low-energy interactions between the quasiparticles are determined by the static Bose propagators R^p. For instance, the phase velocity fluctuations $i\tilde{r}\dot{\theta}$ couple to $f_m^{\dagger p}f_m^{\pm p}$, and thereby induce an interaction

$$\hat{H}_{ff}=-\frac{1}{N}\sum\sum_{p,s=\pm m,m'}\left[\frac{1}{\tilde{r}_0^2}R^s_{\dot{\theta}\dot{\theta}}(0)f_m^{+p}f_{m'}^{+p'}f_{m'}^{p's}f_m^{ps}\right]. \tag{4.37}$$

This is a repulsive interaction, because $(1/\hat{r}_0^2)R_{\dot{\theta}\dot{\theta}}(0)\sim-\tilde{\Delta}$, as verified from the one-impurity results (3.73). To remain general we shall also consider the interactions that mix f and conduction electrons. The full fluctuation $\bar{\mathbf{r}}^s=(\delta\tilde{r}^s,i\tilde{r}\dot{\theta}^s)$ $(s=\pm)$ couples to the Fermion bilinear

$$\mathcal{J}_m^{p,s}=\left[\tilde{r}_0^{-1}f_m^{\dagger p}f_m^{sp},\sum_k V^p(k)(c_{km}^{\dagger p}f_m^{ps}+f_m^{\dagger ps}c_{km}^p)\right] \tag{4.38}$$

through the interaction $N\Sigma_{P,m}\bar{\mathbf{r}}^s(\tau)\cdot\mathcal{J}_m^{p,s}(\tau)$. Upon integrating out the Bose fluctuations, the zero frequency components of the Bose propagators mediate the following interaction

$$\hat{H}_{\rm int}=\frac{1}{2N}\mathcal{T}\left[\sum\sum_{s,p,p'=\pm m,m'}\mathcal{J}_m^{p,s}\cdot\mathbf{R}^s(0)\mathcal{J}_{m'}^{p',s}\right], \tag{4.39}$$

where $\mathcal{T}$ orders the fermion operators to eliminate any potential scattering,

$$\mathcal{T}[(\psi_a^\dagger\psi_b)(\psi_c^\dagger\psi_d)]=\psi_a^\dagger\psi_c^\dagger\psi_d\psi_b\ . \tag{4.40}$$

When we introduce a quasiparticle of parity p, spin m we modify the static value of $\langle\mathcal{J}_m^{p,+}\rangle$ causing a shift in

the saddle point and a change in the mean-field scattering potential. We shall denote these changes in the f occupation and mixing by the vector

$$\bar{\mathbf{j}}^p_m = \delta\langle \mathcal{J}^{p,+}_m \rangle \ . \tag{4.41}$$

This vector acts as a source current which couples to the Bose field, inducing a change in the mean-field values.

Now the change in the ground-state energy per additional quasiparticle with energy label ε (the energy of the corresponding scattering state in the absence of the local scattering potential) near the Fermi energy is given by the scattering phase shift

$$\delta E^p_{qp} = \left[\varepsilon - \frac{1}{\pi\rho}\delta^p(\varepsilon) \right] \delta n^p_m(\varepsilon) \ . \tag{4.42}$$

The expectation values of the two components of $\langle \mathcal{J}^{p,+}_m \rangle$ (mixing and f occupation, respectively) are given by the derivative of the ground-state energy with respect to $\tilde{r}_0 \tilde{E}_f$ and $\tilde{r}$ respectively, so the current $\bar{\mathbf{j}}^p_m$ is determined by the corresponding derivative of δE^p_{qp},

$$\bar{\mathbf{j}}^p_m = \left[\frac{\partial}{\partial \tilde{r}_0}, \frac{1}{\tilde{r}_0}\frac{\partial}{\partial \tilde{E}_f} \right] \delta E^p_{qp} = \frac{\rho^p}{\rho \tilde{r}_0}(-2\tilde{E}^p_f, 1)\delta n^p_m \ , \tag{4.43}$$

where we have substituted $\delta^p = \tan^{-1}(\tilde{\Delta}^p/\tilde{E}^p_f)$ for the phase shift in order to carry out the differential. $\rho^p = (\pi)^{-1}\tilde{\Delta}^p/[(\tilde{\Delta}^p)^2 + (\tilde{E}^p_f)^2]$ is the quasiparticle density of states in the channel with parity p.

We now wish to calculate the energy of interaction between quasiparticles. To do this we require the correction to the ground-state energy that is second order in δn^p_m. The interaction energy is computed using the interaction (4.39) to calculate the Hartree-Fock correction to the ground-state energy caused by the change in the f occupation and mixing.

There are two contributions to the interaction energy. The first is mediated by the symmetric fluctuations, and is given by

$$\delta E^{(+)}_{\rm int} = -\frac{1}{2} \sum_{(p,m)\neq(p',m')} \bar{\mathbf{j}}^p_m \cdot \mathbf{R}^{(+)}(0) \cdot \bar{\mathbf{j}}^{p'}_{m'} \ . \tag{4.44}$$

Terms involving equal parity and spin do not appear because the direct contribution is exactly cancelled by the exchange. The second interaction term is mediated by the antisymmetric fluctuations. These do not couple directly to $\bar{\mathbf{j}}^p_m$, but they do couple via the exchange or Fock term, giving a contribution

$$\delta E^{(-)}_{\rm int} = \frac{1}{2} \sum_{(p,m)} \bar{\mathbf{j}}^p_m \cdot \mathbf{R}^{(-)}(0) \cdot \bar{\mathbf{j}}^{-p}_m \ . \tag{4.45}$$

Only states of equal spin couple in the exchange term.

Finally, inserting (4.45) into (4.24) and (4.45) yields

$$\delta E^{(+)}_{\rm int} = -(\pi\rho)^{-1} \sum_{(p,m)\neq(p',m')} \Phi^{(+)}_{pp'} \delta n^p_m \delta n^{p'}_{m'} \ , \tag{4.46}$$

$$\delta E^{(-)}_{\rm int} = (\pi\rho)^{-1} \sum_{p,m} \Phi^{(-)}_{p,-p} \delta n^p_m \delta n^{-p}_m \ , \tag{4.47}$$

where

$$\Phi^{(s)}_{pp'} = -\frac{\pi\rho^p\rho^{p'}}{N\tilde{r}^2_0\rho}[4\tilde{E}^p_f E^{p'}_f R^{(s)}_{rr} - 2(\tilde{E}^p_f + \tilde{E}^{p'}_f)R^{(s)}_{r\dot{\theta}} + R^{(s)}_{\dot{\theta}\dot{\theta}}] \ . \tag{4.48}$$

The total energy change up to second order in δn^p_m is then given by $\delta E = \Sigma_p \delta E^p_{qp} + \delta E^p_{\rm int}$. Following Noziéres,[6] we shall summarize these results by writing the shift in the ground state energy in terms of an occupation dependent phase shift, given by

$$\frac{\delta E}{\delta n^p_m(\varepsilon)} = \varepsilon - \frac{1}{\pi\rho}\delta^p(\varepsilon, n^{p'}_{m'}) \ , \tag{4.49}$$

where

$$\delta^p_m(\omega, n^{p'}_{m'}) = \delta^p_m(\omega) + \sum_{(p',m')\neq(p,m)} \Phi^{(+)}_{pp'} n^{p'}_{m'} - \Phi^{(-)}_{p-p} n^{(-p)}_m \ , \tag{4.50}$$

where n^p_m is the number of additional quasiparticles of spin m, parity p. In the limit $R \to \infty$, $\Phi(+) - \Phi(-) \to 0$ and this reverts to the one impurity Nozières result.

The quasiparticle interactions corresponding to this Fermi-liquid relation are

$$\hat{H}_{\rm int} = \tfrac{1}{2} I^+ \sum_{(p,m)\neq(p',m')} \hat{n}^p_m n^{p'}_{m'} - I^- n^p_m n^{-p}_m \ , \tag{4.51}$$

where $I^{\pm} = [\rho/\rho^p\rho^{p'}\pi]\Phi^{\pm}_{pp'}$ and n^p_m are the number of quasiparticles of parity p, spin m, energy ε (close to the Fermi energy). I^+ and I^- are the direct and exchange interactions between the quasiparticles. The spatial extent of the Fermi liquid now splits the degeneracy between the direct and exchange terms. Figure (14) plots these interactions for two cases. For the weakly quenched regime we find $I^- - I^+ < 0$ corresponding to a "ferromagnetic" or attractive triplet interaction between the quasiparticle states of opposite parity. For the strongly quenched case we find that $I^- - I^+ > 0$, or antiferromagnetic intersite interactions. This result is fully consistent with the sign of the intersite susceptibilities calculated in these two cases.

We note finally, that in the Kondo regime the Wilson ratio $W = \tilde{\chi}/\tilde{\gamma}$ is modified by the exchange interaction. It is straightforward to show that *quite generally,* independent of our mean field theory, the Wilson ratio is given by

$$W = \frac{N}{(N-1)}\left[1 + \frac{(\Phi^{(+)}_{+-} - \Phi^{(-)}_{+-})\rho}{[\delta'^{(+)}(0) + \delta'^{(-)}(0)]} \right] \ . \tag{4.52}$$

The departure from the one impurity value is plotted in Fig. 15.

V. STRONG COUPLING IN THE LATTICE

Extension of our analysis of fluctuations to a lattice model involves no new formal complications. Unlike the approaches which explicitly constrain fluctuations in Q

via the Abrikosov trick, or via Keiter Kimball perturbation theory,[49,10,11,9] the broken symmetry approach does *not* get more and more complicated as one adds additional ions, and provides a well defined prescription for modeling the lattice. In the fluctuations, the Q conservation symmetry insures that

$$\langle \delta q(\mathbf{R}_1,\tau)\delta q(\mathbf{R}_2,0)\rangle = 0 \ . \tag{5.1}$$

Now of course, the analysis is aided by defining Bose fluctuations with a definite wavelength

$$\delta\tilde{r}(\mathbf{q},\tau)=\frac{1}{(N_{\text{sites}})^{1/2}}\sum_{\mathbf{R}_j}\delta\tilde{r}(\mathbf{R}_j,\tau)e^{-i\mathbf{q}\cdot\mathbf{R}_j} \ ,$$

$$\dot{\theta}(\mathbf{q},\tau)=\frac{1}{(N_{\text{sites}})^{1/2}}\sum_{\mathbf{R}_j}\dot{\theta}(\mathbf{R}_j,\tau)e^{-i\mathbf{q}\cdot\mathbf{R}_j} \ . \tag{5.2}$$

Lattice momentum is conserved in the interactions, and the quadratic terms in the effective free-energy functional are diagonal in this momentum representation of the fluctuations,

$$\beta\Omega_{\text{eff}}=\beta\Omega_0+N\int\frac{d^3q}{(2\pi)^3}\sum_{i\nu_n}\delta\mathbf{r}^T(\mathbf{q},i\nu_n)\Gamma(q,i\nu_n)\delta\mathbf{r}(\mathbf{q},i\nu_n) \ , \tag{5.3}$$

where, now,

$$\Gamma(\mathbf{q},i\nu_n)=2\begin{bmatrix}\lambda_0 & 1\\ 1 & 0\end{bmatrix}+\Pi(\mathbf{q},i\nu_n) \tag{5.4}$$

and the polarization graphs involve a sum over the wave vectors and frequencies of the internal electron lines. Once we have determined the mean-field propagators, we can determine the RPA polarization diagrams,

$$\begin{aligned}
\Pi_{rr}(\mathbf{q},\tau)&=\tilde{r}_0^{-2}\int\frac{d^3q}{(2\pi)^3}[2G_{fb}(\mathbf{k}+\mathbf{q},\tau)G_{fb}(\mathbf{k},-\tau)+G_b(\mathbf{k}+\mathbf{q},\tau)G_f(\mathbf{k},-\tau)+G_f(\mathbf{k}+\mathbf{q},\tau)G_b(\mathbf{k},-\tau)] \ ,\\
\Pi_{r\dot{\theta}}(\mathbf{q},\tau)&=\tilde{r}_0^{-2}\int\frac{d^3q}{(2\pi)^3}[G_{fb}(\mathbf{k}+\mathbf{q},\tau)G_f(\mathbf{k},-\tau)+G_f(\mathbf{k}+\mathbf{q},\tau)G_{fb}(\mathbf{k},-\tau)] \ ,\\
\Pi_{\dot{\theta}\dot{\theta}}(\mathbf{q},\tau)&=\tilde{r}_0^{-2}\int\frac{d^3q}{(2\pi)^3}[G_f(\mathbf{k}+\mathbf{q},\tau)G_f(\mathbf{k},-\tau)] \ ,
\end{aligned} \tag{5.5}$$

where

$$\begin{aligned}
G_f(\mathbf{k},\tau)&=\langle Tf_m(\mathbf{k},\tau)f^{\dagger}m(\mathbf{k},0)\rangle \ ,\\
G_{fb}(\mathbf{k},\tau)&=\sum_{\mathbf{k}}\tilde{V}(\mathbf{k}+\mathbf{G})\langle Tf_m(\mathbf{k},\tau)c_m^{\dagger}(\mathbf{k}+\mathbf{G},\tau)\rangle \ ,\\
G_b(\mathbf{k},\tau)&=\sum_{\mathbf{k},\mathbf{G},\mathbf{G}'}\tilde{V}(\mathbf{k}+\mathbf{G})\tilde{V}(\mathbf{k}+\mathbf{G}')\langle Tc_m(\mathbf{k}+\mathbf{G},\tau)c_m^{\dagger}(\mathbf{k}+\mathbf{G}',\tau)\rangle \ ,
\end{aligned} \tag{5.6}$$

and the sum is over reciprocal lattice vectors $\mathbf{G}$. Determination of correlations and interactions in the strong coupling regime hinges on the determination of the matrix $\Pi(\mathbf{q},i\nu_n)$. In a similar fashion to the two impurity model the high-frequency behavior of $\Gamma(\mathbf{q},\nu)$ will be independent of wave vector $\mathbf{q}$ due to the local character of the high frequency fluctuations. However, the interesting physics of the lattice problem lies in the low-frequency fluctuations, and these have momentum dependences that reflect the lattice symmetry.

In the Cartesian gauge we know that the Q conservation symmetry will lead to a zero mode at each wave vector. This feature spells disaster for any attempt to use a renormalization-group analysis to study strong coupling features of the lattice, for this would require keeping track of at least one relevant Kondo coupling constant $J(\mathbf{k})$ for *each* momentum $\mathbf{k}$.

The outlook for an accurate numerical treatment of the Bose fluctuations in the lattice is optimistic, and some initial studies are underway.[50–52] As in the two-impurity model, the hybridization with higher bands will affect results quite dramatically through the f-band dispersion, and the inclusion of this dispersion is an important part of the calculation.

Evidently, once we have determined the polarization matrix, we can immediately determine the spin and the charge susceptibilities. The momentum-dependent dynamic spin susceptibility is determined from

$$\tilde{\chi}(\mathbf{q},\omega)=-\frac{1}{\tilde{r}_0^2}\Pi_{\dot{\theta}\dot{\theta}}(\mathbf{q},\omega) \ . \tag{5.7}$$

If we integrate over the $\mathbf{q}$ dependence of $\Pi(\mathbf{q},\nu)$, this theory will predict a spin susceptibility rather similar to the one-impurity result, with a quasielastic peak for filling factors less than half and a Lorentzian peak for a filling factor $q=\frac{1}{2}$.

Particularly interesting however, will be the momentum dependence of the spin susceptibility which we expect to be quite marked at temperatures $T\ll\tilde{\Delta}$ and frequencies $\omega\ll\tilde{\Delta}$, with the interesting possibility of spin correlations being strongly dependent on filling factor, as in the two-impurity model.

The second aspect of heavy fermion systems where we expect this approach to be useful is in the modeling of Fermi-liquid properties. Given $\mathbf{R}(\mathbf{q},\omega=0)$ we can determine the low energy interactions between electrons. For

instance the direct f-f interaction between quasiparticles will be

$$\hat{H}_{ff}=\frac{1}{2}\sum_{\mathbf{q}} I(\mathbf{q}) \sum_{\substack{\mathbf{k},\mathbf{k}' \\ m,m'}} f_m^\dagger(\mathbf{k}+\mathbf{q}) f_{m'}^\dagger(\mathbf{k}') f_{m'}(\mathbf{k}'-\mathbf{q}) f_m(\mathbf{k}) , \tag{5.8}$$

where $I(\mathbf{q})=-(1/N\tilde{r}_0^2)R_{\dot{\theta}\dot{\theta}}(\mathbf{q},\omega=0)$, with two other interaction terms coupling to the mixing matrix elements. From these interaction terms one extracts the A_n^l interaction parameters of the Fermi liquid. The momentum dependence of $\mathbf{R}(\mathbf{q})$ is of particular interest to any calculation of the triplet interaction strength between quasiparticles, which depends on a dipole component of $\mathbf{R}(\mathbf{q})$. As in the two-impurity case, filling factor will play a crucial role in the sign of these interactions.

Various authors[53–55] have compared heavy Fermion systems with the Brinkman-Rice picture of ^{3}He, with almost localized quasiparticles. It is clear that in our model the interactions will be weakly momentum dependent because of the very weak momentum dependence of the quasiparticle dispersion, and it is therefore correct to think of these quasiparticles as almost localized. However, the two-band structure with interactions propagating through both amplitude (hybridization) and phase fluctuations (f-level position) in the mean-field potential indicate that we are dealing with more degrees of freedom than in a simple one-band picture, and close analogies between ^{3}He and heavy fermion systems may be misleading.

Whilst the leading interactions contain a $O(1/N)$ prefactor, we should not attach too much significance to this prefactor. We are not attempting to gain a quantitatively accurate model of real systems from the leading Gaussian fluctuations, but rather by organizing our calculation as a $1/N$ expansion about a broken symmetry limit we are provided with a consistent model with many of the properties we associate with mixed-valence systems. Thus we should not regard the leading interactions as small, but rather, as providing a guide to the qualitative properties of the interactions, and their dependence on physically important quantities (such as the filling factor q) in the finite degeneracy system. Of course some systems do have large spin degeneracies in their ground states, (such as YbCuAl, $CePd_3$), and in these cases we have some hope of gaining quantitative accuracy. In other systems, such as those with twofold ground-state degeneracies, we aim to gain a guide to the strong-coupling properties from this model.

In the lattice there will be a close relationship between the Bose fluctuations and the transport properties. In our semiclassical picture of mixed valence, as we raise the temperature, the electrons involved in conduction sample an increasing amount of the high-frequency fluctuations, which will inelastically scatter the electrons and lead to a rapid rise in the resistivity from zero in the Fermi-liquid regime. Investigations into the inelastic scattering generated by the fluctuations are now in progress.

Another aspect of mixed valence properties which this approach lends itself to is the introduction of phonons. One of the controversial issues about heavy-fermion systems is the question of whether phonons are involved in the mediation of heavy-fermion superconductivity. Fulde, Razamafimandimby, and Grewe[56,57] have proposed models of phonon-mediated superconductivity in heavy-fermion systems, but little detailed thought has been put into the interplay between Coulomb and phonon interactions in these systems. Very clearly, the small charge susceptibility of the f electrons makes direct coupling to the f electrons a very unlikely contender for a pairing mechanism, for if the bare coupling to a local phonon, ϕ, has the form

$$\hat{H}=g\phi\hat{n}_f , \tag{5.9}$$

then at the mean-field level, we deduce the renormalized coupling to be

$$\hat{H}=g\phi\tilde{\chi}_c\left[\hat{n}_f-\sum_{km}\frac{V(k)}{r_0}(c_{km}^\dagger f_m+\text{H.c.})\right] , \tag{5.10}$$

where

$$\tilde{\chi}_c=\Delta^{-1}\text{Im}\left[1+\frac{\Delta}{\xi}\right]^{-1}\sim(\tilde{\Delta}/\Delta)=\tilde{r}_0^2 ,$$

which is tiny when the system is in the Kondo regime. If we were dealing with a one-band system this would rule out phonon mediated superconductivity when the band structure is very narrow. However, this does not rule out coupling to the band electrons, which at the mean-field level is unrenormalized, or coupling to the hybridization matrix element, which is only weakly renormalized. It seems an interesting question to see how the Fermi-liquid properties are modified by introducing such couplings, leading to a dynamical interplay between the phonon and "slave-boson" fluctuations. This is particularly interesting when the phonon frequencies are comparable with the heavy bandwidth.

A. Introduction of a realistic angular momentum structure

A wide variety of experiments show the Fermi-liquid properties of narrow band f-electron systems to be highly anisotropic, and clearly, the use of a realistic lattice structure and realistic angular momentum structure is needed to model these properties. Our quasiclassical treatment of mixed valence readily generalizes to incorporate both of these features. When we have spin-half-band electrons hybridizing with spin-orbit coupled, large degeneracy f electrons, the hybridization takes the form

$$\hat{H}_{\text{mix}}=\sum_{\sigma=\pm\frac{1}{2},\mathbf{R},\mathbf{k},m}\frac{V(k)}{\sqrt{N}}[c_{k\sigma}^\dagger f_m(\mathbf{R})b^\dagger(\mathbf{R})e^{-i\mathbf{k}\cdot\mathbf{R}}Y_{l,m-\sigma}(\hat{\mathbf{k}})(jl\tfrac{1}{2};m\mid l,m-\sigma;s=\tfrac{1}{2},\sigma)+\text{H.c.}] , \tag{5.11}$$

where l ($=3$ typically) is the orbital angular momentum of the f state and j ($=3\pm\frac{1}{2}$ typically) is the total angular

momentum of the spin-orbit coupled f state. When we compute the saddle-point equations the mean-field behavior is determined by a hybridization term of the form

$$\hat{H}_{\rm mix}=\sum \tilde{V}(k)[c^{\dagger}_{\mathbf{k}\sigma}f_m(\mathbf{R})e^{-i\mathbf{k}\cdot\mathbf{R}}Y_{l,m-\sigma}(\hat{\mathbf{k}})(jl\tfrac{1}{2};m\mid l,m-\sigma;\tfrac{1}{2}\sigma)+\text{H.c.}]\ , \tag{5.12}$$

where $\tilde{V}(k)=V(k)\tilde{r}_0$ is the renormalized hybridization. Using this mixing we compute $\tilde{E}_f=E_f+\lambda$ self-consistently from

$$\tilde{E}_f=E_f-\frac{1}{N\tilde{r}_0^2}\sum_{\mathbf{k},\mathbf{G},m}\tilde{V}(\mathbf{k}+\mathbf{G})\langle c^{\dagger}_{\mathbf{k}+\mathbf{G}m}f_m(\mathbf{k})\rangle Y_{l,m-\sigma}(\mathbf{k})(jl\tfrac{1}{2};m\mid l,m-\sigma;\tfrac{1}{2}\sigma) \tag{5.13}$$

and

$$q_0=\tilde{r}_0^2+\frac{1}{N}\sum_{k,m}\langle f^{\dagger}_m(\mathbf{k})f_m(\mathbf{k})\rangle\ . \tag{5.14}$$

These self-consistency conditions can be built into a KKR band-structure calculation in a very straightforward fashion. Given the renormalized band structure from such a calculation, it is straightforward to determine the polarizabilities $\Pi(\mathbf{q},i\nu_n)$ from which the dynamic susceptibilities and the Fermi-liquid properties can be evaluated in the Gaussian approximation. Crystal-field splitting of the f levels into multiplets can also be simply added to the model, and its effect on the mean-field properties is closely akin to a magnetic field. Local crystal fields strongly effect the effective ground-state spin degeneracy, modifying the magnetic moments and Sommerfeld ratio of the Fermi liquid.

B. Further generalizations

Our approach of treating the strong-coupling regime of an electronic system as an almost broken symmetry can be further generalized. The simplest generalization is made by introducing one extra boson field $\hat{a}$ (per site) to model high-frequency charge fluctuations into a doubly occupied state with energy $2E_f+U$. The additional terms

$$\hat{H}_i=\sum_{k,m}V(k)(c^{\dagger}_{km}f_m a^{\dagger}+af^{\dagger}_m c_{km})+(2E_f+U)a^{\dagger}a \tag{5.15}$$

are then added to the Hamiltonian.

The formally correct way to add a second boson would be to use the coupling to $\sum_{k,m}V(k)\{c^{\dagger}_{km}f^{\dagger}_{-m}a+\text{H.c.}\}$, since destruction of the doubly occupied state leads to formation of two fermions. This version was proposed by Barnes a decade ago[58,59] for modeling the symmetric Anderson model. Unfortunately, any attempt to treat this boson model in a mean field leads to anomalous "pairing" terms which destroy fermion conservation at the mean-field level and introduce a spurious gap into the excitation spectrum.

The coupling (5.15) avoids this problem, but is only valid when the "a" boson amplitude is very small, corresponding to occasional virtual scattering into the doubly occupied state. This extension is therefore a method of introducing the leading spin-fluctuation corrections of large but finite U. The conserved quantity Q is now given by $Q=a^{\dagger}a+b^{\dagger}b+\hat{n}_f$ and the corresponding symmetry is given by $f\to fe^{i\theta},b\to be^{i\theta},a\to ae^{i\theta}$. The second Bose field represents the charge degree of freedom associated with doubly occupied state of energy $2E_f+U$. If we take $N\to\infty$ with $q=Q/N$ finite, we find a meanfield broken symmetry solution. At $T=0$ the mean-field equations are simply

$$\tilde{E}_f=E_f^{*}+\frac{\Delta}{\pi}\left[\frac{\tilde{E}_f+U}{E_f+\tilde{E}_f+U}\right]\ln\left[\frac{\Delta}{\pi(\tilde{E}_f^{\,2}+\tilde{\Delta}^{\,2})^{1/2}}\right]\ ,$$

$$\tilde{a}^{\,2}+\tilde{b}^{\,2}+\frac{1}{\pi}\tan^{-1}\left[\frac{\tilde{\Delta}}{\tilde{E}_f}\right]=q_0\ , \tag{5.16}$$

$$\tilde{a}=[(\tilde{E}_f-E_f)/(E_f+\tilde{E}_f+U)]\tilde{b}\ ,$$

where $\tilde{\Delta}=\Delta[\tilde{a}^{\,2}+\tilde{b}^{\,2}]$ and $\tilde{a}=\langle a\rangle/\sqrt{N}$, $\tilde{b}=\langle b\rangle/\sqrt{N}$. In the Kondo limit where $\tilde{E}_f\ll\Delta$, we find $\tilde{E}_f+i\tilde{\Delta}=T_K e^{i\pi q_0}$, where $T_K=De^{-1/J\rho}$ and

$$J\rho=\frac{\Delta}{E_f+U}-\frac{\Delta}{E_f} \tag{5.17}$$

is the well-known Schrieffer-Wolffe expression for the Kondo coupling constant.

Another generalization can be made by applying this approach to the infinite-U Hubbard model, writing

$$\hat{H}=\sum_{i,j,m}t_{ij}[(b_i c^{\dagger}_{im}c_{jm}b^{\dagger}_j)+(a_i c^{\dagger}_{im}c_{jm}a^{\dagger}_j)]+\sum_i Ia^{\dagger}_i a_i \tag{5.18}$$

which for $N=2,Q=1$ is equivalent to the infinite-U Hubbard model. The Bose fields used here are dynamical, unlike those employed in a conventional Hubbard-Stratonovich transformation. Unfortunately, as in the Anderson model, we run into problems with fermion conservation at the mean-field level when we try to model double occupation and finite U by a second boson, and so far as is known, more than two Bose fields are required.[37]

VI. SUMMARY

We have attempted to present, in as much detail as possible, a new approach for modeling strong coupling in mixed-valence and Kondo systems. The essence of our approach has been to incorporate the strong correlations intrinsic to strong coupling as an underlying symmetry. The large degeneracy limit of the model can then be solved exactly, and yields a broken-symmetry mean-field solution at low temperatures which contains crucial nonperturbative effects of strong coupling, including the formation of narrow extended heavy Fermion bands. By carrying out a semiclassical expansion in the fluctuations about this broken-symmetry state we are able to con-

sistently model the strong-coupling behavior in a way which preserves the symmetries associated with the constraint. The singular properties of the strong coupling regime are incorporated through the broken symmetry, and strong coupling in mixed valence and the Kondo problem is viewed as arising from critical zero-mode fluctuations about an almost-broken-symmetry state.

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APPENDIX A: CALCULATION OF RPA DIAGRAMS IN SINGLE-IMPURITY MODEL

We wish to evaluate the Matsubara sums

$$\Pi_{rr}=\beta^{-1}\sum_n G_f(i\omega_n+i\nu_n)G_f(i\omega_n)\times[\alpha(i\omega_n,i\nu_n)]^2+\Gamma(i\nu_n)\ ,$$
$$\Pi_{r\dot\theta}=(\beta\tilde r_0)^{-1}\sum_n G_f(i\omega_n+i\nu_n)G_f(i\omega_n)\alpha(i\omega_n,i\nu_n)\ , \quad \text{(A1)}$$
$$\Pi_{\dot\theta\dot\theta}=(\beta\tilde r_0^2)^{-1}\sum_n G_f(i\omega_n+i\nu_n)G_f(i\omega_n)\ ,$$

where

$$\alpha(i\omega_n,i\nu_n)=\tilde r_0[\Sigma_f(i\omega_n)+\Sigma_f(i\omega_n+i\nu_n)]\ ,$$
$$\Gamma(i\nu_n)=\beta^{-1}\sum_n G_f(i\omega_n)[\Sigma_f(i\omega_n-i\nu_n)+\Sigma_f(i\omega_n+i\nu_n)]$$
$$=2\,\mathrm{Re}\left[\beta^{-1}\sum_n G_f(i\omega_n)\Sigma_f(i\omega_n-i\nu_n)\right]\ , \quad \text{(A2)}$$

and the propagators are defined as in Sec. II C. To evaluate these sums we convert them to a contour integral around the poles of the Fermi function $f(\omega)$. In the large-bandwidth limit,

$$G_f(z)=1/[z-\tilde E_f+i\,\mathrm{sgn}(z_I)\tilde\Delta]\ , \quad \text{(A3)}$$

where $z_I=\mathrm{Im}z$ and for $\nu_n>0$ we have

$$\alpha(z,i\nu_n)=\begin{cases}-2i\tilde r_0\Delta, & \mathrm{Im}z>0\\ 0, & -\nu_n<\mathrm{Im}z<0\\ 2i\tilde r_0\Delta, & \mathrm{Im}z<-\nu_n\ .\end{cases} \quad \text{(A4)}$$

Deforming the contour integral around the two branch cuts at $\mathrm{Im}z=0$ and $-\nu_n$ then gives

$$\beta^{-1}\sum_n G_f(i\omega_n+i\nu_n)G_f(i\omega_n)[\alpha(i\omega_n,i\nu_n)]^m=\sum_{P=\pm1}\int_{-\infty}^{\infty}\frac{dx}{\pi}f(x)\mathrm{Im}\{G_f(x-i\delta)G_f(x+Pi\nu_n)[\alpha(x-i\delta,Pi\nu_n)]^m\} \quad \text{(A5)}$$

and

$$\Gamma(i\nu_n)=2\int_{-\infty}^{\infty}\frac{dx}{\pi}f(x)\tilde\Delta\mathrm{Re}[G_f(x+i\nu_n)-G_f(x-i\delta)]\ . \quad \text{(A6)}$$

By using the result

$$\int_{-\infty}^{\infty}\frac{dx}{\pi}\phi(x/D)f(x)\frac{1}{x-z}=\frac{1}{\pi}\left[\tilde\psi(z)-\ln\frac{D\beta}{2\pi i}\right] \quad \text{(A7)}$$

for a Lorentzian band cutoff $\phi(x)=(1+x^2)^{-1}$ of width D, we then arrive at the result

$$\Pi_{rr}=\frac{4\tilde\Delta}{\nu_n}\mathrm{Re}\frac{\Delta}{\pi}[\tilde\psi(\xi+i\nu_n)-\tilde\psi(\xi)]+\Gamma(i\nu_n)\ ,$$
$$\Pi_{r\dot\theta}=\frac{2}{\nu_n}\mathrm{Im}\frac{\Delta}{\pi}[\tilde\psi(\xi+i\nu_n)-\tilde\psi(\xi)]\ , \quad \text{(A8)}$$
$$\Pi_{\dot\theta\dot\theta}=\frac{-2}{\nu_n(\nu_n+2\tilde\Delta)}\mathrm{Re}\frac{\Delta}{\pi}[\tilde\psi(\xi+i\nu_n)-\tilde\psi(\xi)]\ ,$$

where

$$\Gamma(i\nu_n)=2\,\mathrm{Re}\frac{\Delta}{\pi}[\tilde\psi(\xi+i\nu_n)-\tilde\psi(\xi)]+\frac{2\Delta}{\pi}\left[\tilde\psi(\xi)-\ln\left[\frac{D\beta}{2\pi}\right]\right]\ . \quad \text{(A9)}$$

For $\nu_n<0$ the result is obtained from the complex conjugate of these results. These are the results quoted in (3.47).

APPENDIX B: EVALUATION OF FLUCTUATIONS IN THE CARTESIAN GAUGE

Here we show the equivalence of the Gaussian fluctuations in the Cartesian-Bose coordinates to the fluctuations already determined in the radial coordinate systems for the Bose field. In the Cartesian coordinates, the Gaussian correction to the free energy is

$$\beta F_g = N\sum_{i\nu_n}\bar{b}(i\nu_n)b(i\nu_n)[\lambda - i\nu_n + \Pi_0(i\nu_n)] + \frac{N}{2}\sum_{i\nu_n}[\bar{b}(i\nu_n)\bar{b}(-i\nu_n)+b(i\nu_n)b(-i\nu_n)]\Pi_A(i\nu_n)\ , \tag{B1}$$

where $\Pi^0(i\nu_n)$ is the "normal" Bose self-energy and $\Pi^A(i\nu_n)$ is the anomalous self-energy generated by the finite amplitude of the Bose field. The expressions for these self-energies are then

$$\Pi_0(i\nu_n) = (\beta)^{-1}\sum_{i\nu_n} G_f(i\omega_n + i\nu_n)[\Sigma_f(i\omega_n) + \tilde{r}_0^2\Sigma_f^2(i\omega_n)G_f(i\omega_n)]$$

$$\Pi_A(i\nu_n) = \frac{\tilde{r}_0^2}{\beta}\sum_{i\nu_n} G_f(i\omega_n + i\nu_n)G_f(i\nu_n)\Sigma_f(i\omega_n)\Sigma_f(i\omega_n + i\nu_n) \tag{B2}$$

and by carrying out the Matsubara frequency sums we find

$$\Pi_0(i\nu_n) = \left[\frac{\Delta}{\pi}[\tilde{\psi}(\xi + i\nu_n) - \tilde{\psi}(\xi)]\right]^* + \left[\frac{2\tilde{\Delta}^2}{\nu_n(\nu_n + 2\Delta)}\right]\mathrm{Re}\frac{\Delta}{\pi}[\tilde{\psi}(\xi + i\nu_n) - \tilde{\psi}(\xi)] + \frac{\Delta}{\pi}\mathrm{Re}\left[\tilde{\psi}(\xi) - \left[\ln\frac{D\beta}{2\pi i}\right]\right],$$

$$\Pi_A(i\nu_n) = \frac{\tilde{\Delta}(\tilde{\Delta} + \nu_n)}{\nu_n(\nu_n + \tilde{\Delta})} 2\,\mathrm{Re}\frac{\Delta}{\pi}[\tilde{\psi}(\xi + i\nu_n) - \tilde{\psi}(\xi)]\ . \tag{B3}$$

Now if we write $b_x(i\nu_n) = b_x(i\nu_n) + ib_y(i\nu_n)$ where b_x and b_y are real fields, then writing $\bar{s}(i\nu_n) = (b_x(i\nu_n), ib_y(i\nu_n))$, we discover that

$$\beta F_g[b(i\nu_n), b_y(i\nu_n)] = \sum_{i\nu_n}\bar{s}^{\dagger}(i\nu_n)\Gamma_{\mathrm{Cart}}(i\nu_n)\bar{s}(i\nu_n) \tag{B4}$$

where $\bar{s}^{\dagger}(i\nu_n) = [\bar{s}^*(i\nu_n)]^T = (b_x^*(i\nu_n), -ib_y^*(i\nu_n))^T$ and the matrix $\Gamma_{\mathrm{Cart}}(i\nu_n)$ is given by

$$\Gamma_{\mathrm{Cart}}(i\nu_n) = \begin{bmatrix} \lambda + \Pi_A(i\nu_n) + \mathrm{Re}\Pi_0(i\nu_n) & -i\nu_n + i\,\mathrm{Im}\Pi_0(i\nu_n) \\ -i\nu_n + i\,\mathrm{Im}\Pi_0(i\nu_n) & \lambda - \Pi_A(i\nu_n) + \mathrm{Re}\Pi_0(i\nu_n) \end{bmatrix}. \tag{B5}$$

In the two diagonal terms of Γ_{Cart} we can use the saddle-point condition $\lambda + \Delta/\pi\,\mathrm{Re}[\tilde{\psi}(\xi) - \ln(D\beta/2\pi i)] = 0$ to eliminate the explicit dependence on λ. Inserting the results (B4) yields

$$\Gamma_{\mathrm{Cart}}(i\nu_n) = \begin{bmatrix} \dfrac{1}{g(i\nu_n)}\mathrm{Re}\mathscr{L}(i\nu_n) & -i\,\mathrm{Im}\mathscr{L}(i\nu_n) \\ -i\,\mathrm{Im}\mathscr{L}(i\nu_n) & g(i\nu_n)\mathrm{Re}\mathscr{L}(i\nu_n) \end{bmatrix}, \tag{B6}$$

where $g(i\nu_n)$ and $\mathscr{L}(i\nu_n)$ were defined in (3.48). Had we taken the result from radial coordinates and recognized that $\delta b_y(\tau) = \tilde{r}_0\delta\theta(\tau)$ so that $(-i\nu_n)i\delta b_y(i\nu_n) = i\tilde{r}_0\theta(i\nu_n)$, then by putting

$$\Gamma_{\mathrm{Cart}}(i\nu_n) = \begin{bmatrix} \Gamma_{rr} & -i\nu_n\Gamma_{r\dot{\theta}} \\ -i\nu_n\Gamma_{r\dot{\theta}} & (-i\nu_n)^2\Gamma_{\dot{\theta}\dot{\theta}} \end{bmatrix} \tag{B7}$$

and using (3.50) we obtain identical results to (B6) above, showing the equivalence of leading fluctuations in the two-coordinate systems for the one-impurity model.

APPENDIX C: IMPOSITION OF CONSTRAINT FOR AN ARRAY OF MAGNETIC SITES

Consider an array of magnetic sites at positions $\mathbf{R}_j$. To generate the correlation functions for $Q_i(\tau), n_f(\mathbf{R}_i,\tau)$ and $r_i^2(\tau)$ the source term

$$\beta F_s = \sum_i \int_0^\beta d\tau\{\zeta_i(\tau)[Q_i(\tau) - Q_0] + \phi_i(\tau)n_f(\mathbf{R}_i,\tau) + j_i(\tau)r_i^2(\tau)\} + \int_0^\beta d\tau\sum_\alpha J_\alpha(\tau)O_\alpha(\tau) \tag{C1}$$

is added to the free-energy functional, where the currents $\zeta_i(\tau)$, $\phi_i(\tau)$, $j_i(\tau)$, and $J_\alpha(\tau)$, are external sources. The additional source terms coupling to the operators O_α allow us to discuss cross correlations with other variables of interest. We are working in the radial gauge of Newns and Read.

The effective thermodynamic potential Ω_{eff}, determined by

$$e^{-\beta\Omega_{\mathrm{eff}}} = \int \mathscr{D}[r,\dot{\theta},\bar{\psi},\psi]e^{-\beta(F+F_s)} \tag{C2}$$

then generates correlation functions of interest, for instance,

$$\langle T\delta Q_i(\tau)\delta n_f(\mathbf{R}_j,0)\rangle = -\frac{\delta^2\beta\Omega_{\rm eff}}{\delta\zeta_i(\tau)\delta\phi_j(0)} ,$$

$$\langle T\delta Q_i(\tau)\prod_{\alpha}^{n-1}\delta O_\alpha(\tau_\alpha)\rangle = -\prod_\alpha \frac{\delta}{\delta\zeta_i(\tau)}\frac{\delta}{\delta J_\alpha(\tau)}\beta\Omega_{\rm eff} , \tag{C3}$$

where the prefix δ denotes fluctuation from the mean, for instance, $\delta Q_i(\tau)=Q_i(\tau)-Q_0$.

In the radial gauge, the constraint on $Q_i(\tau)$ is imposed through the terms $i\dot\theta_i(\tau)[Q_i(\tau)-Q_0]$ in the free-energy functional. Now in the path integral, the measure for angular velocity fluctuations is linear $\mathscr{D}[\dot\theta]=\Pi_\tau d\dot\theta(\tau)$.

Under the translation in $\dot\theta$,

$$\dot\theta_i'(\tau)=\dot\theta_i(\tau)-i[\zeta_i(\tau)+\phi_i(\tau)] , \tag{C4}$$

the measure is unchanged, whilst the source currents $\zeta_i(\tau)$ are entirely absorbed into the constraint. The source term now becomes

$$\beta F_s' = \sum_i \int_0^\beta d\tau[j_i(\tau)-\phi_i(\tau)]r_i^2(\tau) - Q_0\int_0^\beta d\tau\sum_i\phi_i(\tau) \tag{C5}$$

Consequently, $\Omega_{\rm eff}$ is independent of $\zeta_i(\tau)$ and all correlation functions (C3) involving fluctuations in $Q_i(\tau)$ vanish.

These statements remain true when the path integral over r and $\dot\theta$ is approximated by the leading Gaussian corrections to mean-field theory, as will be shown below. In general, after integrating out the Fermions in the path integral, the Gaussian approximation to the bose effective action is

$$\beta F_{\rm eff} = N\sum_{i,j,i\nu_n}[\bar{\mathbf{r}}_j(-i\nu_n)+\boldsymbol{\mathscr{f}}_j(-i\nu_n)]\boldsymbol{\Gamma}_{jk}(i\nu_n)[\bar{\mathbf{r}}_k(i\nu_n)+\boldsymbol{\mathscr{f}}_k(i\nu_n)]+N\sum_{j,i\nu_n}\mathbf{r}_j(-i\nu_n)\mathbf{S}_j(\tau)(i\nu_n)$$
$$+N\sum_j[j_i(i\nu_n)\langle r_i^2\rangle+\phi_i(i\nu_n)\langle n_f(\mathbf{R}_i)\rangle]_{i\nu_n=0} , \tag{C6}$$

where $\mathbf{R}_j(i\nu_n)=[\delta\tilde r_j(i\nu_n),i\tilde r_{0j}\dot\theta_j(i\nu_n)]$($\tilde r_{0j}=\langle\tilde r_j\rangle_{\rm MFT}$ is the mean-field value of $\tilde r_j$ and the currents shown are

$$\boldsymbol{\mathscr{f}}_j(i\nu_n)=[\phi_j(i\nu_n)+\zeta_j(i\nu_n)](0,-i\tilde r_{0j}^{-1}) ,$$
$$\mathbf{S}_j(i\nu_n)=[j_j(i\nu_n)+\zeta_j(i\nu_n)](2\tilde r_{0j},0) . \tag{C7}$$

The additional source terms coupling to O_α have been temporarily omitted.

The gaussian integral runs from $-\infty$ to ∞ in r_j and $\dot\theta_j$ with linear measures in both variables,

$$e^{-\beta\Omega_{\rm eff}}=e^{-\beta\Omega_{\rm MFT}}\int\prod dR_j(i\nu_n)d\dot\theta_j(i\nu_n)e^{-\beta F_{\rm eff}} . \tag{C8}$$

At this stage we note that *without* further approximation, the linear translation of $\dot\theta_j$ can be carried out, preserving the gaussian form of the free energy. Writing this translation of variables in Fourier transformed variables

$$i\dot\theta_j'(i\nu_n)=i\dot\theta_j(i\nu_n)+\{\zeta_j(i\nu_n)+\phi_j(i\nu_n)\} \tag{C9}$$

then yields

$$\beta F_{\rm eff}=N\sum_{j,k,i\nu_n}\bar{\mathbf{r}}_j(-i\nu_n)\boldsymbol{\Gamma}_{jk}(i\nu_n)\bar{\mathbf{r}}_k(i\nu_n)+N\sum_{j,i\nu_n}2\tilde r_{0j}\delta r_j(-i\nu_n)[j_i(i\nu_n)-\phi_i(i\nu_n)]$$
$$+N\sum_j[j_j(i\nu_n)-\phi_j(i\nu_n)]_{i\nu_n=0}r_{0j}^2 . \tag{C10}$$

So even within the Gaussian approximation, the path integral is independent of source terms coupling to the charges Q_j.

If we reintroduce the additional couplings $J_\alpha(\tau)O_\alpha(\tau)$ to the original free-energy functional, then at the Gaussian level, this adds additional linear and quadratic terms to the free-energy functional, but, providing that none of the O_α depend on $\dot\theta_j$, then these additional source terms do not introduce any dependence on ζ_j. This means that the full generating functional computed to Gaussian order $\Omega_{\rm eff}[\zeta_i,j_i,\phi_i',J_\alpha]$ is independent of ζ_j so that the correlations involving fluctuations in $\hat Q_j(\tau)$ identically vanish. So quite generally, the constraint is imposed consistently in the leading Gaussian fluctuations.

Furthermore, the dependence on $j_i(i\nu_n)$ and $\phi_j(i\nu_n)$ only enters in the combination $j_i(i\nu_n)-\phi_i(i\nu_n)$, so that the f occupation and Bose fluctuations are precisely anticorrelated,

$$\left\langle T\delta r_j^2(\tau)\prod_{\alpha=1}^n\hat O_\alpha(\tau_\alpha)\right\rangle = -\left\langle T\delta n_f(\mathbf{R}_j,\tau)\prod_{\alpha=1}^n\delta\hat O_\alpha(\tau_\alpha)\right\rangle . \tag{C11}$$

We wish to dwell on this result for the particularly interesting case when the source terms couple directly to Fermi fields. Consider the general fermion source term

$$\beta F_{\psi s}=\sum_{\alpha,m}\int_0^\beta d\tau[\bar\eta_{\alpha m}(\tau)\psi_{\alpha m}(\tau)+\bar\psi_{\alpha m}(\tau)\eta_{\alpha m}(\tau)] , \tag{C12}$$

where the $\bar\eta_{\alpha m}$ and $\eta_{\alpha m}$ are conjugate Grassman variables.[43] When the fermion fields are integrated away, this adds the additional term

$$\beta F_{\psi\text{eff}} = \int_0^\beta d\tau\, d\tau' \bar{\eta}_{\alpha m}(\tau) G_{\alpha\beta}(\tau,\tau';\delta\bar{\mathbf{r}}_i)\eta_{\beta m}(\tau') \tag{C13}$$

to βF_{eff}, where $G_{\alpha\beta}(\tau,\tau';\delta\bar{\mathbf{r}}_i) = \langle T\psi_{\alpha m}(\tau)\psi^\dagger_{\beta m}(\tau')\rangle$ is the propagator for electrons moving in the field of the bosons. To Gaussian order in the fluctuations,

$$\begin{aligned} G_{\alpha\beta}(\tau,\tau';\delta\bar{\mathbf{r}}) = G_{\alpha\beta}(\tau-\tau') &+ \int_0^\beta d\tau_1 G_{\alpha\gamma}(\tau-\tau_1)[\bar{\mathbf{\Lambda}}^j_{\gamma\eta}\cdot\delta\bar{\mathbf{r}}_j(\tau_1)]G_{\eta\beta}(\tau_1-\tau') \\ &+ \int_0^\beta d\tau_1 d\tau_2 G_{\alpha\gamma}(\tau-\tau_1)[\bar{\mathbf{\Lambda}}^j_{\gamma\eta}\cdot\delta\bar{\mathbf{r}}_j(\tau_1)]G_{\eta\sigma}(\tau_1-\tau_2)[\bar{\mathbf{\Lambda}}^j_{\sigma\mu}\cdot\delta\bar{\mathbf{r}}_j(\tau_2)]G_{\mu\beta}(\tau_2-\tau')\ , \end{aligned} \tag{C14}$$

where the $\bar{\Lambda}^i_{\alpha\beta}$ are the vertices coupling the electrons to the Bose field at site i and the Green's functions $G_{\alpha\beta}(\tau-\tau')$ are the mean-field propagators for the fermions. The important point is that there is no new ζ_j dependence introduced by the Fermion source terms. This means in particular, that when we do the final Gaussian integral over the Bose fields, the final generating functional $\Omega_{\text{eff}}[\zeta_i,\bar{\eta}_i,\eta_i]$ is independent of ζ_i, so that by differentiating with respect to source currents we find that

$$\left\langle T\delta Q_j(\tau)\prod_{i=1}^n \psi^\dagger_{\alpha_i m_i}(\tau_i)\prod_{j=1}^n \psi_{\beta_j m_j}(\tau_j)\right\rangle = 0\ . \tag{C15}$$

The corollary to this result, first shown by Read in the case of one impurity,[39] is that for any two states of quasiparticles $|\alpha\rangle$ and $|\beta\rangle$,

$$\begin{aligned} \langle\alpha|\hat{Q}_j|\beta\rangle - Q_0\langle\alpha|\beta\rangle &= \langle 0|T\prod_\alpha \psi_\alpha(0^+)\delta\hat{Q}_j(0)\prod_\beta \psi^\dagger_\beta(0^-)|0\rangle \\ &= 0 \end{aligned} \tag{C16}$$

where $|0\rangle$ is the ground state. This nontrivial result within the Gaussian approximation is consistent with the expectation that the quasiparticles do not carry the "charges" Q, and further evidence that the constraint is consistently imposed at the gaussian level of approximation. In the Kondo limit $Q = n_f$, so in this limit the quasiparticles do not carry f-charge n_f, even though the quasiparticle band forms from resonances in the f channel.

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