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Odd-frequency pairing in the Kondo lattice

P. Coleman and E. Miranda
Serin Physics Laboratory, Rutgers University, P.O. Box 849, Piscataway, New Jersey 08855

A. Tsvelik
Department of Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, United Kingdom
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We discuss the possibility that heavy-fermion superconductors involve odd-frequency triplet pairing. A key technical innovation here is a Majorana representation for the local moments which avoids the use of a Gutzwiller projection. We employ the Kondo lattice model and develop a mean-field theory for odd-frequency pairing that entails pairing between local moments and conduction electrons, as described by a spinor order parameter. We confirm that the Meissner stiffness is positive and the state is stable. A residual band of gapless quasiparticles whose spin and charge coherence factors vanish *linearly* in energy, decouples from the condensate. The unusual energy dependence of these coherence factors leads to a T^3 NMR relaxation rate at a conduction electron site that coexists with a linear specific heat. Two verifiable predictions of the theory are (i) that a Korringa relaxation will fail to develop in heavy-fermion superconductors, even in the limit of strong pair breaking and severe gaplessness and (ii) that the hitherto unmeasured NMR relaxation rate at the actinide or rare-earth site will become exponentially activated in the superconducting phase.

I. INTRODUCTION

Heavy-fermion superconductivity has attracted great interest in recent years as a candidate for electronically mediated pairing.[1] Six heavy-fermion metals are superconducting at room pressure: $CeCu_2Si_2$,[2] UBe_{13},[3] UPt_3,[4] URu_2Si_2,[5] UNi_2Al_3, and UPd_2Al_3.[6] These metals contain a dense array of magnetic rare-earth or actinide ions that collectively participate in the formation of the superconducting state. Many properties set these systems apart from traditional superconductors. In particular, power laws in the specific heat, thermal conductivity, NMR relaxation rate, and acoustic attenuation all point to the existence of gap nodes, and have been interpreted in terms of gap zeros along lines of the Fermi surface. Furthermore, each of these superconductors appears to coexist with some measure of antiferromagnetic order.[7]

Existing phenomenological models of heavy-fermion superconductivity treat it as a pairing process involving the performed heavy f quasiparticles.[8–12] The strong repulsive interactions between these f quasiparticles favor the development of nodes in the pair wave function, as suggested by the preponderance of power laws. Theoretical work on heavy-fermion superconductivity has focused largely on the possibility of momentum anisotropy in the gap function $\Delta_{\mathbf{k}}$ as the origin of this node formation. The simplest candidates for gap functions with nodes are odd-parity triplet pairing, $\Delta_{\mathbf{k}}=-\Delta_{-\mathbf{k}}$, or even-parity d-wave pairing. Two points appear to favor the latter possibility.

(1) d-wave pairing is favored by the antiferromagnetic interactions that are characteristic to heavy-fermion compounds.[8,13]

(2) lines of gap zeros inferred from many power-law properties of the condensed state, e.g., T^3 dependence of the NMR relaxation rate, T^2 dependence of specific heat, and thermal conductivity, effectively rule out triplet odd-parity pairing. Simple symmetry arguments show that odd-parity triplet would give rise to a gap vanishing at points, rather than lines on the Fermi surface, in the presence of strong spin-orbit scattering.[10,14]

Unfortunately, there are several observations that do not fit naturally into the d-wave scenario. One puzzling observation is the persistence of the T^3 NMR relaxation rate in heavy-fermion superconductors with very large densities of gapless excitations and correspondingly "heavy" linear components to their specific heat.[15,16] This gaplessness has been attributed to pair breaking by resonantly scattering off nonmagnetic defects.[17] Remarkably, this constant density of quasiparticle states does not seem to give rise to an observable Korringa NMR relaxation. In UPt_3 and $U_{1-x}Th_xBe_{13}$, for example,[15,16] the linear specific heat is of the same order as the normal phase value, yet there are more than two decades[18,19] of T^3 spin relaxation:

$$\left.\frac{C_v}{T}=\gamma+BT\right\}\text{linear term from pair breaking ,}$$

$$\vdots \tag{1.1}$$

$$\left.\frac{1}{T_1T}=?+DT^2\right\}\text{no linear term from pair breaking?}$$

In conventional gapless superconductivity,[20–22] spin coherence factors are unity at the Fermi energy. The robustness of the T^3 NMR signal suggests vanishing spin-coherence factors: a feature not easily accommodated by a conventional pairing hypothesis.

The d-wave scenario is also unable to explain the isotropy of the H-T phase diagram of UPt_3.[12,23] UPt_3 has *three* separate low-temperature flux phases that have been interpreted in terms of anisotropic pairing. There is a two-stage phase transition at zero field associated with the symmetry-breaking effects of the weak heavy-fermion antiferromagnetism, and perhaps also, a recently discovered incommensurate charge-density wave.[24] The *d*-wave scenario supposes a gap function that transforms under a two-dimensional representation of the point group: though this picture can account for the two-stage transition, it predicts a two-phase flux lattice for all orientations of the applied field.[25]

Finally, of course, the *d*-wave pairing picture of heavy-fermion superconductivity makes no reference to the close link between heavy-fermion superconductivity and magnetism. Typically, the entropy associated with the superconducting phase,

$$S_{sc}=\int_0^{T_c} dT\frac{C_V(T)}{T}=C_V[T_c]|_n , \tag{1.2}$$

is a significant proportion of the $R\ \ln 2$ entropy associated with the quenching of the low-lying doublets: in this sense heavy-fermion superconductivity is a *spin-ordering* process, involving the magnetic, rather than the charge degrees of freedom of the f electrons. In most cases, heavy-fermion superconductivity appears to coexist with antiferromagnetic order.[7] In the recently discovered 1-2-3 compound UPd_2Al_3, an ordered moment of $0.8\mu_B$ coexists[26] with the superconductivity. In URu_2Si_2, there is also evidence for a large moment–free order parameter that breaks time-reversal and translation symmetries.[27,28] Unlike the well-known Chevrel phases,[29] this moment shares the same magnetic degrees of freedom that are involved in pairing. It is rather difficult to account for coexistent magnetism and superconductivity in terms of two weakly coupled order parameters.

These difficulties motivate us to reconsider the way in which heavy-fermion superconductors develop nodes in the pair wave function. Past analyses of heavy-fermion superconductivity have focused on the spatial anisotropy. In this paper we explore a new avenue, examining the possibility of pair condensation into a state where the pair wave function has *odd* temporal parity.[30–33] In this hypothetical state, pairing is retarded and the pair wave function contains a *node in time.*[34]

Berezinskii[30] first pointed out that a general pairing hypothesis must consider the symmetry of the pair wave function under frequency inversion. Let us denote the pair wave function

$$[\underline{F}(\kappa)]_{\alpha\beta}=\langle \psi_\alpha(\kappa)\psi_\beta(-\kappa)\rangle . \tag{1.3}$$

Here $\langle \cdots \rangle$ denotes the time-ordered expectation value, and we use a four-vector notation $\kappa\equiv(\mathbf{k},\omega)$. Since the Fermi operators anticommute, the pair wave function satisfies

$$\underline{F}(\kappa)=-\underline{F}^T(-\kappa) , \tag{1.4}$$

where $[\underline{F}^T]_{\alpha\beta}=[\underline{F}]_{\beta\alpha}$ denotes the wave function with spin indices transposed. Now if we assume that the state breaks neither time-reversal symmetry, nor spatial parity, then the pair wave function must have distinct spatial, temporal, and spin parity. Let $(S,P,T=\pm1)$ be the parities of the pair wave function under the interchange of spin, space, or time coordinates, respectively, i.e.,

$$\underline{F}(\mathbf{k},\omega)=\begin{cases} S\underline{F}^T(\mathbf{k},\omega) \\ P\underline{F}(-\mathbf{k},\omega) \quad (S,P,T=\pm1) , \\ T\underline{F}(\mathbf{k},-\omega) \end{cases}$$

then the total antisymmetry of the pair wave function implies that the combined product of all three parities must equal -1:

$$SPT=-1 . \tag{1.5}$$

Superconductors with an antisymmetric spin wave function, $S=-1$ are "singlet" superconductors,

$$\underline{F}(\kappa)=i\underline{\sigma}_2F_s(\kappa) \quad (\underline{F}=-\underline{F}^T) , \tag{1.6}$$

whereas superconductors with a symmetric spin wave function, $S=+1$ are "triplet"

$$\underline{F}(\kappa)=i\underline{\sigma_2\sigma}\cdot\mathbf{F}_t(\kappa) \quad (\underline{F}=+\underline{F}^T) . \tag{1.7}$$

In conventional superconductivity $T=+1$ so that the spatial parity of singlet and triplet states is even and odd, respectively. Berezinskii has argued that symmetry also permits the possibility of odd-frequency pairing where

$$T=-1 ,\qquad P=\begin{cases} +1 \quad (\text{triplet } \{S,P,T\}=\{+,+,-\}) , \\ -1 \quad (\text{singlet } \{S,P,T\}=\{-,-,-\}) . \end{cases} \tag{1.8}$$

Odd-frequency, *even-parity,* triplet pairing was first considered by Berezinskii in the context of He-3. A renaissance of interest in these types of states has been prompted by the work of Balatsky and Abrahams, who are the first to discuss the possibility of odd-frequency, *odd-parity,* singlet pairing.[31]

Historically, odd-frequency pairing has not enjoyed a great deal of attention. One reason for this lack of attention is that the simplest odd-frequency paired state is *unstable,* with a negative Meissner phase stiffness. For example, in the s-wave triplet state $(S,P=+1)$ the momentum dependence of the gap function vanishes, and the London kernel is formally identical to s-wave singlet pairing

$$\Lambda=\frac{\pi Ne^2T}{m}\sum_{\omega_n^2+\Delta_n^2>0}\frac{\Delta_n^2}{(\Delta_n^2+\omega_n^2)^{3/2}} \quad [\Delta_n=\Delta(i\omega_n)] . \tag{1.9}$$

Since an odd gap function where $\Delta_n=-\Delta_{-n}$ must also satisfy the analyticity requirement $\Delta_n=\Delta^*_{-n}$, this implies Δ_n is purely imaginary. Thus, $\Delta_n^2<0$ and the stiffness is negative. The negative phase stiffness indicates that the microscopic phase of the order parameter likes to "coil up." In our simple model for odd-frequency pairing, the condensation energy reaches a minimum in a staggered phase configuration: loosely speaking, the Josephson coupling of the phase at neighboring sites has the opposite sign to conventional superconductors and the screening currents vanish when the microscopic phase is staggered.

We shall argue that the Kondo effect between a conduction sea and local moments in heavy-fermion metals provides an ideal source of retarded scattering for odd-frequency pairing. In the normal state, this retardation generates resonant bound states between the conduction electrons and local moments, quenching the moments and forming the heavy quasiparticles. In the superconducting state, the resonant Kondo scattering acquires a pairing component that results in even-parity, odd-frequency triplet pairing of the conduction electrons. This state develops a phase stiffness by the simultaneous condensation of the local moments and the conduction electron pair degrees of freedom. The equal time order parameter is a matrix correlating these two degrees of freedom:

$$\langle \tau_\alpha(x) S^\beta(x) \rangle = g \underline{\mathcal{M}}^\beta_\alpha(x) \quad (\alpha,\beta=1,2,3) . \tag{1.10}$$

Here $\mathbf{S}[x_j]$ denotes the local moment spin at site j; $\tau[x]$ is the conduction electron "isospin," whose z component describes the number density, and transverse components describe the pairing

$$\tau_3 = \tfrac{1}{2}[\rho(x)-1] , \tag{1.11}$$

$$\tau_+(x) = \psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x) . \tag{1.12}$$

The quantity g defines the magnitude of the order parameter. $\underline{\mathcal{M}}$ is an orthogonal matrix whose rows define an orthogonal triad of unit vectors $\hat{d}_\lambda$,

$$\underline{\mathcal{M}}(x) = \begin{bmatrix} \hat{d}_1(x) \\ \hat{d}_2(x) \\ \hat{d}_3(x) \end{bmatrix} . \tag{1.13}$$

A "composite" order parameter of this form has been recently suggested as an order parameter for odd-frequency pairing in the context of the two-channel Kondo model, by Emery and Kivelson.[32] We shall show within our model that a uniform pairing field configuration is unstable and that the Josephson coupling energy is minimized for a *staggered* composite order parameter: in our simple model the screening currents vanish when $\hat{d}_1$ and $\hat{d}_2$ are staggered commensurately with the lattice.

Within our theory, the microscopic manifestation of this type of pairing is an anomalous self-energy in the triplet channel with a pole at zero frequency:

$$\underline{\Delta}(\kappa) = i\sigma_2 \underline{d}_c \left[\frac{V^2}{2\omega} \right] \quad (\underline{d}_c = [\hat{d}_1 + i\hat{d}_2]\cdot\sigma) . \tag{1.14}$$

A spinless component of the conduction electron band decouples from this singular pairing field, giving rise to surfaces of gapless excitations. Spin and charge coherence factors of these quasiparticles vanish linearly with the energy on the Fermi surface,

$$\left.\begin{matrix} \langle \mathbf{k}'|\rho_{\mathbf{k}-\mathbf{k}'}|\mathbf{k}\rangle \\ \langle \mathbf{k}'|S^z_{\mathbf{k}-\mathbf{k}'}|\mathbf{k}\rangle \end{matrix}\right\} \propto \omega \quad (\omega = E_{\mathbf{k}'} + E_{\mathbf{k}}) , \tag{1.15}$$

creating the unusual circumstance where a flow of quasiparticles transmits heat without passage of charge or spin. Vanishing coherence factors are, of course, well known in BCS superconductivity, where at the gap energy the charge coherence factor vanishes. The odd-frequency character of the triplet superconductor shifts the energy scale at which coherence factors vanish to zero energy.

These unusual coherence factors lead to a T^3 dependence of the nuclear magnetic relaxation rate of the conduction electrons

$$\left.\frac{1}{T_1}\right|_{\text{cond}} \propto T^3 . \tag{1.16}$$

Unlike d-wave superconductivity, this power-law dependence is a matrix element effect, and coexists with a constant quasiparticle density of states and linear specific heat. By contrast, our theory predicts a *gap* in the f-electron excitation spectrum that would manifest itself as an exponential nuclear relaxation rate at the "heavy-fermion" actinide or rare-earth site

$$\left.\frac{1}{T_1 T}\right|_f \propto \exp[-\Delta_g/T] . \tag{1.17}$$

NMR relaxation experiments on the rare-earth or actinide site have yet to be made, due to perceived difficulties in resolving broadened nuclear line widths. This pairing scenario predicts that in the superconducting state an exponential reduction in the NMR relaxation rate at the heavy-fermion site will make it possible to resolve the NMR line at low temperatures (Fig. 1).

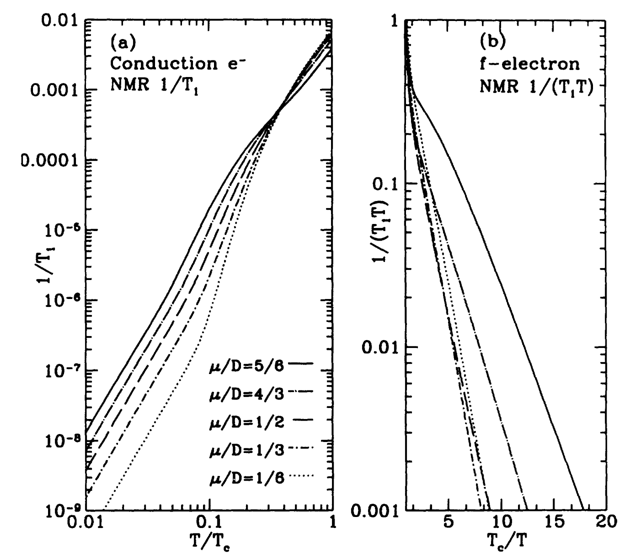


FIG. 1. Showing (a) conduction electron NMR relaxation rate, and (b) f-spin relaxation rate computed using our toy model for a sequence of μ/D values. Even though the model predicts a linear specific heat (Fig. 8), the coherence factors give rise to a conduction electron NMR relaxation rate normally associated with lines, rather than surfaces of gapless excitations. There is no Hebel-Slichter peak below the mean-field transition temperature. By contrast, the relaxation rate at the heavy-fermion site is entirely exponential, reflecting the "s-wave" character of the odd-frequency paired state.

An essential part of our analysis is a second quantized description of the local moments that avoids constraints. Existing treatments factorize the spin variable in terms of spin-$\frac{1}{2}$ fermions:

$$\mathbf{S}=f^{\dagger}_{\alpha}\left[\frac{\boldsymbol{\sigma}}{2}\right]_{\alpha\beta}f_{\beta}\ . \tag{1.18}$$

This approach requires a constraint $n_f=1$ to impose the condition $S=\frac{1}{2}$, which is the origin of additional complications. In many practical applications, the constraint is weakened, imposing it at the mean field or the Gaussian level of approximation. Here, we employ real, or "Majorana" fermions to represent spins. Perhaps the most famous example of a Majorana fermion is a single Pauli spin operator. Recall that

$$\{\sigma_a,\sigma_b\}=2\delta_{ab} \tag{1.19}$$

so the fermions

$$\boldsymbol{\eta}=\frac{1}{\sqrt{2}}\boldsymbol{\sigma} \tag{1.20}$$

also satisfy a canonical anticommutation algebra $\{\eta_a,\eta_b\}=\delta_{ab}$. Indeed, for *any* such triplet of Majorana fermions, it follows that the "spin operators"

$$\mathbf{S}=-\frac{i}{2}\boldsymbol{\eta}\times\boldsymbol{\eta} \tag{1.21}$$

simultaneously satisfy *both* the spin algebra, *and* the constraint $S^2=\frac{3}{4}$. The generalization of this result to a lattice of spins employs a vector of Majorana fermions $\eta_j^a=(\eta_j^a)^\dagger$ $(a=1,2,3)$ for each site j where

$$\{\eta_i^a,\eta_j^b\}=\delta_{ij}\delta^{ab}\ , \tag{1.22}$$

from which the spin operator at each site is constructed:

$$\mathbf{S}_j=-\frac{i}{2}\boldsymbol{\eta}_j\times\boldsymbol{\eta}_j\ . \tag{1.23}$$

These operators behave as independent spin-$\frac{1}{2}$ operators.

In particle physics, the earliest reference to this method that we know is due to Martin,[35] although earlier references may exist. These results were later developed by Casalbuoni[36] and independently by Berezin and Marinov.[37] In condensed-matter physics, the same method was independently developed under the name "Drone fermion representation," and early mention of this method appears in Mattis' book on magnetism.[38] First application to the Kondo model was made by Spencer and Doniach.[39] The only application of this method to the Kondo lattice model that we are aware of was made by Vieira, who considered the interplay of the Kondo effect and magnetism within this formalism.[40]

The Majorana representation of spins provides a natural lattice generalization of *anticommuting* Pauli operators. On a lattice, we may represent Majorana fermions in terms of a set of $N/2$ independent complex fermions that span half the Brillouin zone (BZ):

$$\boldsymbol{\eta}_j=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}\in 1/2\ \mathrm{BZ}}\{\boldsymbol{\eta}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}_j}+\boldsymbol{\eta}^\dagger_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{R}_j}\}\ . \tag{1.24}$$

These complex fermions obey canonical commutation relations $\{\eta^a_{\mathbf{k}},\eta^{b\dagger}_{\mathbf{k}'}\}=\delta^{ab}\delta_{\mathbf{k}\mathbf{k}'}$; opposite halves of the Brillouin zone are related as complex conjugates: $[\eta^a_{\mathbf{k}}]^\dagger=\eta^a_{-\mathbf{k}}$. Since the Fock space is spanned by $3N/2$ complex Fermi operators, it is $2^{N/2}$ times larger than a Hilbert space of N commuting spin-$\frac{1}{2}$ operators. The spin algebra *and* the condition $S=\frac{1}{2}$ are satisfied between all states of the Fock space, thus the anticommuting representation *replicates* the spin Hilbert space $2^{N/2}$ times.[41] We may then represent the partition function of an electronic system containing N spins as an *unconstrained* trace over the independent Fermi fields

$$Z=\frac{1}{2^{N/2}}\mathrm{Tr}\{e^{-\beta H[\mathbf{S}_j]}\}\ \left[\mathbf{S}_j\to-\frac{i}{2}\boldsymbol{\eta}_j\times\boldsymbol{\eta}_j\right]\ , \tag{1.25}$$

where the formal normalization factor associated with the replication of states has been added.

Our basic model for a heavy-fermion system is an $S=\frac{1}{2}$ Kondo lattice with a single band interacting with one local f moment $\mathbf{S}_j$ in each unit cell. In a real Kondo lattice, the local moments are strongly spin-orbit coupled into a state of definite J. We shall assume that the low-lying spin excitations are described by a Kramers doublet, where a low-energy $S=\frac{1}{2}$ Kondo model becomes more appropriate. For simplicity, we shall ignore the anisotropies that are necessarily present in a real heavy-fermion system. In our model, the latent superconducting pairing is driven by the on-site Kondo interactions, and the state that forms exhibits a coexistence of magnetism and superconductivity.

The simplified isotropic Kondo lattice model that we shall use is then written

$$H=H_c+\sum_j H_{\mathrm{int}}[j]\ , \tag{1.26}$$

where

$$H_c=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}\psi^\dagger_{\mathbf{k}}\psi_{\mathbf{k}} \tag{1.27}$$

describes the conduction band, and $\psi^\dagger_{\mathbf{k}}=(\psi^\dagger_{\mathbf{k}\uparrow},\psi^\dagger_{\mathbf{k}\downarrow})$ is a conduction electron spinor. The exchange interaction at each site j is written in a tight-binding representation as

$$H_{\mathrm{int}}[j]=J(\psi^\dagger_{j\alpha}\boldsymbol{\sigma}_{\alpha\beta}\psi_{j\beta})\cdot\mathbf{S}_j\ . \tag{1.28}$$

When written in terms of the Majorana fermions, this term becomes

$$H_{\mathrm{int}}[j]=-\frac{J}{2}\psi^\dagger_j[\boldsymbol{\sigma}_j\cdot\boldsymbol{\eta}_j]^2\psi_j,\quad \psi_j\equiv\begin{bmatrix}\psi_{j\uparrow}\\ \psi_{j\downarrow}\end{bmatrix}\ , \tag{1.29}$$

where we have used the result $i\boldsymbol{\sigma}\cdot(\boldsymbol{\eta}\times\boldsymbol{\eta})=[\boldsymbol{\eta}\cdot\boldsymbol{\sigma}]^2-\frac{3}{2}$ to simplify the interaction, absorbing the bilinear term as a redefinition of the chemical potential. This simple form of the interaction can be rewritten in a suggestive way, by defining the composite spinor operator

$$\hat{V}_j=\begin{bmatrix}\hat{V}_{j\uparrow}\\ \hat{V}_{j\downarrow}\end{bmatrix}=-\frac{J}{2}[\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_j]\psi_j\ . \tag{1.30}$$

The Kondo interaction is then the "square" of this operator:

$$H_{\text{int}}[j]=-\frac{2}{J}\hat{V}_j^\dagger\hat{V}_j\ , \tag{1.31}$$

suggesting that in the lattice we should consider the possibility of states where the local moment and electron spins condense together to develop a vacuum expectation value of this spinor quantity:

$$\begin{bmatrix}V_{j\uparrow}\\V_{j\downarrow}\end{bmatrix}=\begin{bmatrix}\langle\phi|\hat{V}_{j\uparrow}|\phi\rangle\\\langle\phi|\hat{V}_{j\downarrow}|\phi\rangle\end{bmatrix}\ . \tag{1.32}$$

This order parameter transforms as a spin-$\frac{1}{2}$ object, so changes in its sign correspond to physical rotations of the condensate by 2π. Defects in the spinor field are then disclination lines or "Z_2 vortices," around which the phase of the spinor order parameter changes by π (Fig. 2). The gauge equivalent integral of the vector potential around a Z_2 defect is

$$\frac{e}{\hbar}\int \mathbf{A}\cdot dx=\pi\ , \tag{1.33}$$

so the flux quantum of a "charge e" spinor is the same as a charge "$2e$" scalar:

$$\Phi_0=\int \mathbf{A}\cdot dx=\frac{\hbar}{e}\pi=\frac{h}{2e}\ . \tag{1.34}$$

In our model there is a microscopic "Z_2" gauge symmetry

$$\eta_j\to\pm\eta_j\ . \tag{1.35}$$

V_j transforms in the same way as the Majorana fermions and thus its phase is defined to within $\pm\pi$. Physical quantities involve the combinations of the square of V_j at each site and are Z_2 invariants. The three Z_2 invariant quantities that this defines are just the components of the matrix $\mathcal{M}(x)$:

$$\begin{aligned}&\langle\rho(x)\mathbf{S}(x)\rangle=gV(x)^\dagger\sigma V(x)\ ,\\&\langle\psi_\uparrow^\dagger(x)\psi_\downarrow^\dagger\mathbf{S}(x)\rangle=gV^T(x)i\sigma_2\sigma V(x)\ ,\\&g\equiv\frac{J^2}{2}\ .\end{aligned} \tag{1.36}$$

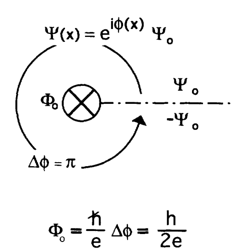


FIG. 2. Illustrating the elementary "Z_2" vortex for a charge e spinor order parameter. Around the vortex, the phase change of the order parameter is π. The supercurrent around this vortex can be removed by introducing a magnetic flux for which $e\Phi/\hbar=(e/h)\int \mathbf{A}\cdot dl=\pi$, so the flux quantum for a charge e spinor is $\Phi=\hbar\pi/e=h/2e$, which corresponds to the flux quantum of a charge $2e$ complex scalar order parameter.

Under a phase change of π in the spinor field, the axes of the composite order parameter rotate through 2π.

The outline of this paper is as follows: Section II deals with the development of a path-integral formulation of the Kondo lattice, demonstrating how the simplest decoupling procedure leads to an odd-frequency paired state, Sec. III is a discussion of the quasiparticle excitations and coherence factors, Sec. IV contains the calculation of the mean-field thermodynamics in this paired state, Sec. V shows the computation of the Meissner stiffness of this phase and the form of the Landau-Ginzburg theory, Sec. VI demonstrates the effect of vanishing coherence factors on local magnetic and charge responses, Sec. VII discusses the interplay with magnetism, and Sec. VIII contains a critique and a discussion of possible application to the theory of heavy-fermion superconductivity.

Readers who are primarily interested in the physical picture that emerges from this approach might find it useful to proceed directly to Sec. VIII, which attempts to place our results in a more general context, beyond the narrow confines of the Kondo lattice model. Certain formal arguments, not pertinent to the main flow of ideas, have been reproduced in the appendices. In Appendix A, we show how the Majorana representation is related to the Abrikosov pseudofermion representation. In Appendix B, we give some examples of the application of the Majorana representation to simple spin models, showing the relation to the Jordan-Wigner transformation in the one-dimensional Heisenberg model.

II. PATH-INTEGRAL REPRESENTATION OF THE KONDO LATTICE MODEL

To develop a "toy model" for the odd-paired state, we focus our attention on a stripped-down Kondo lattice model, with the Hamiltonian described in Eqs. (1.26)–(1.29):

$$H=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}\psi_{\mathbf{k}}^\dagger\psi_{\mathbf{k}}-\frac{J}{2}\sum_j\psi_j^\dagger[\sigma\cdot\eta_j]^2\psi_j\ . \tag{2.1}$$

We have suppressed both the momentum dependence and anisotropy of the coupling. In a real heavy-fermion system, we envisage that the spin indices would refer to the conserved pseudospin indices of the low-lying Kramers doublets.

To illustrate the calculations in this section, we shall use Feynman diagrams, as shown in Fig. 3. The bare propagator for the conduction electrons is represented by a solid arrow, the bare propagator for the Majorana fermions by a dashed line, without an arrow:

$$a\ \text{- - -}\ \kappa\ \text{- - -}\ b\ =\langle\eta^a(\kappa)\eta^b(-\kappa)\rangle_0=\delta^{ab}\left[\frac{1}{i\omega_n}\right]\ ,$$

$$\sigma\ \xrightarrow{\ \kappa\ }\ \sigma'\ =\frac{\delta_{\sigma\sigma'}}{i\omega_n-\epsilon_{\mathbf{k}}}\ . \tag{2.2}$$

The product form of the exchange interaction [Eq. (1.31)] clearly suggests a decoupling in terms of the spinor variable,

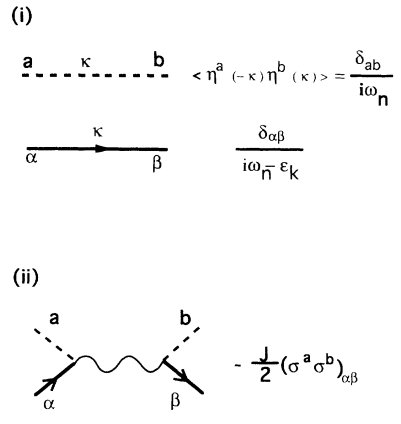


FIG. 3. (i) Bare Majorana and conduction propagators, (ii) interaction between local moment and conduction electrons.

$$V_j=\begin{bmatrix} V_{j\uparrow} \\ V_{j\downarrow} \end{bmatrix} = -\frac{J}{2}\langle [\sigma\cdot\eta_j]\psi_j\rangle \ , \tag{2.3}$$

corresponding to the bound state of an electron and a local moment.

With this point in mind, we now write the partition function as a path integral, $Z=\int_P \exp(-\int_0^\beta \mathcal{L}(\tau)d\tau)$, where

$$\mathcal{L}(\tau)=\sum_{\mathbf{k}}\psi_{\mathbf{k}}^\dagger\partial_\tau\psi_{\mathbf{k}}+\sum_{\mathbf{k}\in\frac{1}{2}\mathrm{BZ}}\eta_{\mathbf{k}}^\dagger\partial_\tau\eta_{\mathbf{k}}+H_c+\sum_j H_{\mathrm{int}}[j] \tag{2.4}$$

and we have factorized the interaction in terms of a fluctuating two-component spinor $V_j^\dagger=(V_\uparrow^*,V_\downarrow^*)$:

$$H_{\mathrm{int}}[j]=\psi_j^\dagger(\sigma\cdot\eta_j)V_j+V_j^\dagger(\sigma\cdot\eta_j)\psi_j+2|V_j|^2/J \ . \tag{2.5}$$

For later purposes, it is particularly useful for us to introduce a Balian-Werthamer four-spinor notation, defining

$$\Psi_j=\begin{bmatrix} \psi_j \\ -i\sigma_2\psi_j^* \end{bmatrix}=\begin{bmatrix} \psi_{j\uparrow} \\ \psi_{j\downarrow} \\ -\psi_{j\downarrow}^\dagger \\ \psi_{j\uparrow}^\dagger \end{bmatrix} ,$$
$$\mathcal{V}_j=\begin{bmatrix} V_j \\ -i\sigma_2V_j^* \end{bmatrix}=\begin{bmatrix} V_{j\uparrow} \\ V_{j\downarrow} \\ -V_{j\downarrow}^* \\ V_{j\uparrow}^* \end{bmatrix} . \tag{2.6}$$

The lower two entries of each spinor are the time-reversed pairs of the upper two entries. In terms of these spinors, the conduction electron Hamiltonian is

$$H_c=\sum_{\mathbf{k}\in\frac{1}{2}\mathrm{BZ}}\Psi_{\mathbf{k}}^\dagger(\epsilon_{\mathbf{k}}-\mu)\underline{\tau}_3\Psi_{\mathbf{k}} \ , \tag{2.7}$$

where

$$(\underline{\tau}_1,\underline{\tau}_2,\underline{\tau}_3)=\left[\left[\begin{array}{c|c} & \underline{1} \\ \hline \underline{1} & \end{array}\right],\left[\begin{array}{c|c} & \underline{i} \\ \hline -\underline{i} & \end{array}\right],\left[\begin{array}{c|c} \underline{1} & \\ \hline & -\underline{1} \end{array}\right]\right] \tag{2.8}$$

denotes the triplet of isospin operators. Note the definition of $\underline{\tau}_2$. The factorized interaction can also be written

$$H_{\mathrm{int}}[j]=\tfrac{1}{2}[\Psi_j^\dagger(\underline{\sigma}\cdot\eta_j)\mathcal{V}_j+\mathcal{V}_j^\dagger(\underline{\sigma}\cdot\eta_j)\Psi_j] + \mathcal{V}_j^\dagger\mathcal{V}_j/J \ , \tag{2.9}$$

where

$$\underline{\sigma}\equiv\sigma\otimes 1=\left[\begin{array}{c|c} \sigma & \\ \hline & \sigma \end{array}\right] \tag{2.10}$$

denotes the spin operator in the Balian-Werthamer notation.

We are particularly interested in expanding around static mean-field configurations where the amplitude of V_j is constant:

$$\mathcal{V}_j=\frac{V}{\sqrt{2}}\mathcal{Z}_j,\quad V_j=\frac{V}{\sqrt{2}}\begin{bmatrix} z_{j\uparrow} \\ z_{j\downarrow} \end{bmatrix} \quad (z_j^\dagger z_j=1) \ , \tag{2.11}$$

where $\mathcal{Z}_j$ is the four-component "unit" spinor

$$\mathcal{Z}_j=\begin{bmatrix} z_j \\ -i\sigma_2 z_j^* \end{bmatrix}=\begin{bmatrix} z_{j\uparrow} \\ z_{j\downarrow} \\ -z_{j\downarrow}^* \\ z_{j\uparrow}^* \end{bmatrix} . \tag{2.12}$$

This choice of mean-field theory is equivalent to a resummation of the interaction lines in the pairing channel between the conduction and Majorana fermions, leading to a saddle-point condition for the anomalous average of Majorana and conduction electrons, as illustrated diagrammatically in Fig. 4(a). The development of this anomalous average leads to self-energy insertions in the conduction electron lines [Fig. 4(b)]. From this diagram, it is evident that the conduction electron self-energies are bilinear forms in the spinor V_j, and are hence *invariant* under the Z_2 gauge symmetry.

We can actually find a class of degenerate mean-field solutions by arbitrarily reversing the sign of $V_j\to m_jV_j$ ($m_j=\pm$) at any site. For each choice of sign, there are $2^{N/2}$ equivalent ways of choosing the independent Majorana creation operators in momentum space ($\eta_{-\mathbf{k}}^\dagger=\eta_{\mathbf{k}}$),

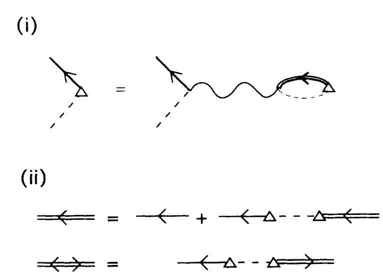


FIG. 4. Diagrammatic illustration of the pairing equations showing (i) the spinor vertex between conduction and Majorana spins, (ii) the self-consistent equation for the conventional and anomalous conduction electron propagators.

there are thus $2^{N-N/2}=2^{N/2}$ independent degenerate saddle-point solutions for each static solution $\{\mathcal{V}_j\}$. Each saddle point is physically identical, so we may absorb the $2^{N/2}$ normalization in the partition function by restricting our attention to one representative saddle point:

$$Z=\frac{1}{2^{N/2}}\sum_{\{m_j\}} Z[\{m\}]=Z[\{m\}]|_{m_j=1} . \tag{2.13}$$

In this way, we fix the gauge for the local Z_2 invariance.

A crucial part of our approach is the stabilization of the odd-frequency paired state through the introduction of a staggered pairing field. Rather than working directly with a staggered order parameter, we may considerably simplify our calculations by making a gauge transformation that absorbs the staggered phase of the order parameter into a redefinition of the conduction electrons. Under the gauge transformation

$$\begin{aligned} z_j&=e^{i(\theta_j/2)}\tilde{z}_j \quad (\mathcal{Z}_j=e^{i(\theta_j/2)\underline{\tau}_3}\tilde{\mathcal{Z}}_j) ,\\ \theta_j&=\mathbf{Q}\cdot\mathbf{R}_j ,\\ \Psi_j&=e^{i(\theta_j/2)\underline{\tau}_3}\tilde{\Psi}_j , \end{aligned} \tag{2.14}$$

the origin of momentum space is shifted by to $\mathbf{k}=\mathbf{Q}/2$. Thus, the conduction electron dispersion transforms $\epsilon_{\mathbf{k}}\to\epsilon_{\mathbf{k}-\mathbf{Q}/2}$. In a Nambu notation, the kinetic energy transforms as $\epsilon_{\mathbf{k}}\to\epsilon_{\mathbf{k}-\mathbf{Q}/2\tau_3}$, or more explicitly

$$\left[\begin{array}{c|c} \epsilon_{\mathbf{k}} & \\ \hline & -\epsilon_{-\mathbf{k}} \end{array}\right]\to\left[\begin{array}{c|c} \epsilon_{\mathbf{k}-\mathbf{Q}/2} & \\ \hline & -\epsilon_{-\mathbf{k}-\mathbf{Q}/2} \end{array}\right] , \tag{2.15}$$

which may be compactly written

$$(\epsilon_{\mathbf{k}}-\mu)\underline{\tau}_3\to\tilde{\epsilon}_{\mathbf{k}}\underline{1}-\mu_{\mathbf{k}}\underline{\tau}_3 , \tag{2.16}$$

where

$$\begin{aligned} \tilde{\epsilon}_{\mathbf{k}}&=\tfrac{1}{2}[\epsilon_{\mathbf{k}-\mathbf{Q}/2}-\epsilon_{\mathbf{k}+\mathbf{Q}/2}] ,\\ \mu_{\mathbf{k}}&=\mu-\tfrac{1}{2}[\epsilon_{\mathbf{k}-\mathbf{Q}/2}+\epsilon_{\mathbf{k}+\mathbf{Q}/2}] . \end{aligned} \tag{2.17}$$

The transformed conduction electron Hamiltonian is then

$$H_c=\sum_{\mathbf{k}\in\frac{1}{2}\mathrm{BZ}}\Psi_{\mathbf{k}}^\dagger[\tilde{\epsilon}_{\mathbf{k}}-\mu_{\mathbf{k}}\underline{\tau}_3]\Psi_{\mathbf{k}} , \tag{2.18}$$

where we have suppressed the tildes on the electron operators. The corresponding matrix propagator for the noninteracting conduction electrons is then

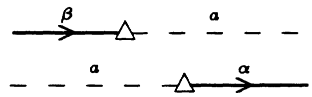
$$=\langle\Psi(\kappa)\Psi^\dagger(\kappa)\rangle_0=[i\omega_n-\tilde{\epsilon}_{\mathbf{k}}+\mu_{\mathbf{k}}\underline{\tau}_3]^{-1} , \tag{2.19}$$

where a bold line is used to indicate the matrix character of the propagator. For a simple bipartite tight-binding lattice, with a commensurate staggered phase, $\mathbf{Q}=(\pi,\pi,\pi)$, then, $\mu_{\mathbf{k}}=\mu$ and $\tilde{\epsilon}_{\mathbf{k}}=\epsilon_{\mathbf{k}-\mathbf{Q}/2}$. With this gauge choice, the conduction electron kinetic energy becomes diagonal in particle-hole space greatly simplifying our work.

The lowest-energy mean-field solution is obtained for a uniformly staggered phase, where $\tilde{\mathcal{V}}_j=\mathcal{V}$ is a constant. With this choice, the admixture between conduction electrons and local moments is described by the mean-field Hamiltonian

$$H_{\mathrm{mix}}=\sum_{\mathbf{k}\in\frac{1}{2}\mathrm{BZ}}[\Psi_{\mathbf{k}}^\dagger(\underline{\sigma}\cdot\eta_{\mathbf{k}})\mathcal{V}+\mathcal{V}^\dagger(\eta_{\mathbf{k}}^\dagger\cdot\underline{\sigma})\Psi_{\mathbf{k}}] . \tag{2.20}$$

In the diagrammatic approach, mixing between the conduction and spin degrees of freedom introduces vertices into the propagators



$$\begin{aligned} &=[\mathcal{V}^\dagger\cdot\underline{\sigma}^a]_\beta ,\\ &=[\underline{\sigma}^a\cdot\mathcal{V}]_\alpha . \end{aligned} \tag{2.21}$$

We may "integrate out" the Majorana fermion degrees of freedom, introducing self-energy diagrams into the conduction electron propagators. An incoming electron which scatters into an intermediate neutral spin state can emerge as a hole, generating both normal and anomalous self-energies, as illustrated in Fig. 4(b). The effective action for the conduction electrons contains this self-energy:

$$S_{\mathrm{eff}}=\sum_{\mathbf{k}\in\frac{1}{2}\mathrm{BZ},\omega=i\omega_n}\Psi^\dagger(\kappa)[\omega-\tilde{\epsilon}_{\mathbf{k}}-\mu_{\mathbf{k}}\underline{\tau}_3-\underline{\Sigma}(\kappa)]\Psi(\kappa) . \tag{2.22}$$

The matrix self-energy $\underline{\Sigma}(\kappa)$ describes the resonant scattering through zero-energy spin states and contains normal and anomalous components. We represent the resonant scattering by the diagram

$$=\left[\frac{1}{i\omega_n}\right]\underline{\sigma}^a\cdot[\mathcal{V}\otimes\mathcal{V}^\dagger]\cdot\underline{\sigma}^a . \tag{2.23}$$

The matrix $\mathcal{V}\otimes\mathcal{V}^\dagger$ can be rewritten

$$\mathcal{V}\otimes\mathcal{V}^\dagger=V^2\underline{p} , \tag{2.24}$$

where

$$[\underline{p}]_{\alpha\beta}=\tfrac{1}{2}\mathcal{Z}_\alpha\mathcal{Z}_\beta^\dagger,\quad(\underline{p}^2=\underline{p}) \tag{2.25}$$

is a projection operator of special significance. By taking the trace of $\underline{p}$ with the matrices $\underline{1}$ and $\sigma^a\otimes\tau^b$, we may expand it in the form

$$\underline{p}=\tfrac{1}{2}[\underline{1}+d_{ab}\sigma^a\otimes\tau^b] , \tag{2.26}$$

where $d_{ab}=\mathrm{Tr}[\underline{p}\sigma^a\otimes\tau^b]=\frac{1}{2}\mathcal{Z}^\dagger\sigma^a\otimes\tau^b\mathcal{Z}$. The columns of the matrix $\underline{d}$ define a triad of orthogonal unit vectors

$$\begin{aligned} [\hat{d}^\lambda]_a&=d_{a\lambda},\ (\lambda=1,2,3)\\ \hat{d}^1+i\hat{d}^2&=z^T(i\sigma_2\sigma)z ,\\ \hat{d}^3&=z^\dagger\sigma z , \end{aligned} \tag{2.27}$$

that determine the spatial orientation of the order parameter. Inserting Eq. (2.26) into Eq. (2.24), we find that the resulting conduction electron self-energy is proportional to $1/\omega$,

$$\underline{\Sigma}(\kappa)=\frac{V^2}{\omega}\underline{\mathcal{P}}\ , \tag{2.28}$$

where the projection operator

$$\underline{\mathcal{P}}=(\underline{1}-\underline{p})=\tfrac{1}{4}[\underline{3}-d_{ab}\sigma^a\otimes\tau^b]\ (\underline{\mathcal{P}}^2=\underline{\mathcal{P}})\ . \tag{2.29}$$

The anisotropic component of the self-energy $-\underline{\Sigma}^{an}(\kappa)=(V^2/4\omega)d_{ab}\sigma^a\otimes\tau^b$ contains "anomalous" components, and may be expanded as

$$\underline{\Sigma}^{an}(\omega)=-\tfrac{1}{2}\left[[\mathbf{B}_j(\omega)\cdot\boldsymbol{\sigma}]\tau_3+[\boldsymbol{\Delta}^\dagger(\omega)\cdot\boldsymbol{\sigma}]\frac{\tau_+}{2}+[\boldsymbol{\Delta}(\omega)\cdot\boldsymbol{\sigma}]\frac{\tau_-}{2}\right]\ . \tag{2.30}$$

We interpret the quantities

$$\begin{aligned}\mathbf{B}(\omega)&=\Delta(\omega)\hat{d}^3\\ \boldsymbol{\Delta}(\omega)&=\Delta(\omega)(\hat{d}^1+i\hat{d}^2)\end{aligned}\quad\left[\Delta(\omega)=\frac{V^2}{2\omega}\right] \tag{2.31}$$

as resonant exchange and triplet pairing fields, respectively. Unlike earlier realizations of odd-frequency pairing,[30,31] here the gap function diverges at zero frequency. Such resonant contributions to the self-energy are well-known within mean-field treatments of the Kondo lattice, but here the resonant scattering acquires additional, anisotropic pairing terms associated with the pair condensate.

The projective form of the pairing self-energy means that only those components of the conduction sea with the same symmetry as the condensate experience the resonance scattering. This leaves behind a residual gapless band of unscattered electrons. This is seen by decomposing the conduction electron operators into four Majorana components

$$\psi_{\mathbf{k}}=\frac{1}{\sqrt{2}}[\psi_{\mathbf{k}}^0+i\boldsymbol{\psi}_{\mathbf{k}}\cdot\boldsymbol{\sigma}]z_o\ . \tag{2.32}$$

The "scalar" component of $\psi_{\mathbf{k}}$

$$\psi_{\mathbf{k}}^0=\frac{1}{\sqrt{2}}\left[z_o^\dagger\psi_{\mathbf{k}}+\psi_{-\mathbf{k}}^\dagger z_o\right]=\frac{1}{\sqrt{2}}Z^\dagger\Psi_{\mathbf{k}} \tag{2.33}$$

so

$$\psi_{\mathbf{k}}^{0\dagger}\psi_{\mathbf{k}}^0=\Psi_{\mathbf{k}}^\dagger\underline{p}\Psi_{\mathbf{k}} \tag{2.34}$$

projects out the scalar component of the conduction sea. The remaining "vector" components of the conduction electron are projected out by the operator $\mathcal{P}=\underline{1}-\underline{p}$.

Projectors $\mathcal{P}$ and $\underline{p}$ select states of the conduction sea where the spin and charge degrees of freedom are locked together to form a hybrid "superspin"

$$Y^a=(\tfrac{1}{2})[\sigma^a-d_{ab}\tau^b]\ . \tag{2.35}$$

Since $\mathbf{Y}_1=\frac{1}{2}\boldsymbol{\sigma}$ and $\mathbf{Y}_2=-\frac{1}{2}\underline{d}\cdot\boldsymbol{\tau}$ are independent spin-$\frac{1}{2}$ degrees of freedom, we may confirm that $\mathcal{P}$ and $\underline{p}$ project out the $Y=1$ and 0 components, respectively:

$$\begin{aligned}&(\text{vector})\ Y=1:\ \mathcal{P}=\tfrac{3}{4}+\mathbf{Y}_1\cdot\mathbf{Y}_2=\tfrac{1}{4}[\underline{3}-d_{ab}\sigma^a\otimes\tau^b]\ ,\\ &(\text{scalar})\ Y=0:\ \underline{p}=\tfrac{1}{4}-\mathbf{Y}_1\cdot\mathbf{Y}_2=\tfrac{1}{4}[\underline{1}+d_{ab}\sigma^a\otimes\tau^b]\ .\end{aligned} \tag{2.36}$$

The vector components of the conduction sea have $Y=1$ whilst the "scalar" components of the conduction sea have $Y=0$. By substituting into the mean-field Hamiltonian, we see that only the vector components of the conduction electrons couple to the resonant scattering potential:

$$H_{\text{mix}}=\sum_{\mathbf{k}\in\frac{1}{2}\text{BZ}}-iV[\boldsymbol{\psi}_{\mathbf{k}}^\dagger\cdot\boldsymbol{\eta}_{\mathbf{k}}-\text{H.c.}]\ . \tag{2.37}$$

Clearly, it is the $Y=1$ electrons that are condensing: these are the electrons with the symmetry of the condensate. We will see shortly that the residual conduction sea that is left behind by this condensation process contains only neutral, spinless excitations, formed from the "scalar" component of the conduction sea.

Further insight into the meaning of the order-parameter matrix $\underline{\mathcal{M}}\equiv\mathcal{V}\otimes\mathcal{V}^\dagger$ is gained by making the identification

$$V_j\equiv-\frac{J}{2}(\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_j)\psi_j \tag{2.38}$$

or

$$\mathcal{V}_j\equiv-\frac{J}{2}(\underline{\boldsymbol{\sigma}}\cdot\boldsymbol{\eta}_j)\Psi_j \tag{2.39}$$

inside the path integral. The expectation value of the matrix $\mathcal{M}$ is then the irreducible part of the corresponding product of operators. In particular,

$$\langle\mathcal{V}_j^\dagger\tau^a\sigma^b\mathcal{V}_j\rangle=\frac{J^2}{4}\langle\Psi_j^\dagger\tau^a(\boldsymbol{\sigma}\cdot\eta_j)\sigma^b(\boldsymbol{\sigma}\cdot\eta_j)\Psi_j\rangle_I\ , \tag{2.40}$$

where "I" denotes the irreducible part. Using the identity $(\boldsymbol{\sigma}\cdot\eta_j)\boldsymbol{\sigma}(\boldsymbol{\sigma}\cdot\eta_j)=[-i\boldsymbol{\eta}_j\times\boldsymbol{\eta}_j-\boldsymbol{\sigma}/2]$ it follows that

$$\langle\mathcal{V}_j^\dagger\tau^a\sigma^b\mathcal{V}_j\rangle=J^2\langle\tau^a[\mathbf{x}_j]S^b[\mathbf{x}_j]\rangle\ , \tag{2.41}$$

where $\mathbf{S}(x_j)\equiv\mathbf{S}_j$ is the local moment at site j and

$$\tau^a[\mathbf{x}]=\tfrac{1}{2}\Psi^\dagger(x)\underline{\tau}\Psi(x) \tag{2.42}$$

is the conduction electron "isospin." This order parameter represents a bound state between the local moments and the conduction electron charge and pair degrees of freedom. The composite order parameter

$$\begin{aligned}\mathbf{d}_c(x)&=\hat{d}^2(x)-i\hat{d}^2(x)\\ &=\frac{2J^2}{V^2}\langle\psi_\downarrow(x)\psi_\uparrow(x)\mathbf{S}(x)\rangle\end{aligned} \tag{2.43}$$

represents the development of a *joint* correlation between the conduction electron singlet pair density and the local moment spin density.[32] Clearly, this state breaks (i) electron gauge symmetry, (ii) spin rotation symmetry and (iii) time-reversal symmetry. Despite these features it does not necessarily follow that the state formed has either an ordered moment, or an equal-time pairing field.

III. EXCITATION SPECTRUM AND QUASIPARTICLES

Let us now examine the nature of the excitation spectrum in this odd-paired state. Let us begin by rewriting the mean-field Hamiltonian in terms of the Majorana components [Eq. (2.32)], then

$$H=\sum_{\mathbf{k}\in\frac{1}{2}\,\mathrm{BZ}} \epsilon_{\mathbf{k}}[\psi_{\mathbf{k}}^{0\dagger}\psi_{\mathbf{k}}^{0}+\boldsymbol{\psi}_{\mathbf{k}}^{\dagger}\cdot\boldsymbol{\psi}_{\mathbf{k}}] -iV[\boldsymbol{\psi}_{\mathbf{k}}^{\dagger}\cdot\boldsymbol{\eta}_{\mathbf{k}}-\mathrm{H.c.}]-\mu n_{\mathbf{k}}\ , \tag{3.1}$$

where

$$n_{\mathbf{k}}=i[\psi_{\mathbf{k}}^{0\dagger}\psi_{\mathbf{k}}^{3}+\psi_{\mathbf{k}}^{1\dagger}\psi_{\mathbf{k}}^{2}-(\mathrm{H.c.})] \tag{3.2}$$

is the total charge operator. Let us consider the special case of $\mu=0$, when the spectrum of the zeroth component remains unrenormalized. In this special case, the Hamiltonian can be written in terms of quasiparticle operators as follows:

$$\begin{aligned} H&=H_o+H_g\ ,\\ H_o&=\sum_{\mathbf{k}\in\frac{1}{2}\,\mathrm{BZ}}\epsilon_{\mathbf{k}}a_{\mathbf{k}0}^{\dagger}a_{\mathbf{k}0}\ ,\\ H_g&=\sum_{\mathbf{k},a=(1,2,3)}E_{\mathbf{k}}a_{\mathbf{k}a}^{\dagger}a_{\mathbf{k}a}\ . \end{aligned} \tag{3.3}$$

The first term describes a gapless "Majorana" conduction band that spans the half of the Brillouin zone where $\epsilon_{\mathbf{k}}>0$. The second term describes a gapped band with excitation energies

$$E_{\mathbf{k}}=\frac{\epsilon_{\mathbf{k}}}{2}\pm\sqrt{(\epsilon_{\mathbf{k}}/2)^2+V^2}\ . \tag{3.4}$$

This band spans the entire Brillouin zone, since it incorporates three Majorana conduction and three Majorana spin fermions. The basic character of the quasiparticle spectrum is unchanged when we consider finite deviations from particle-hole symmetry $\mu_{\mathbf{k}}\neq 0$. There are two important features (Fig. 5).

(1) A threefold degenerate gapful excitation centered around $\mathbf{k}=-\mathbf{Q}/2$. These excitations are formed by the condensation of the "vector" ($Y=1$) component of the conduction sea with the spins. In the vicinity of the gap

$$H_g\sim\sum_{\mathbf{k}\sim-\mathbf{Q}/2,a=(1,2,3)}\left[\Delta_g+\frac{(\mathbf{k}+\mathbf{Q}/2)^2}{m^*}\right]a_{\mathbf{k}a}^{\dagger}a_{\mathbf{k}a}\ , \tag{3.5}$$

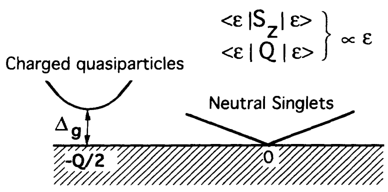


FIG. 5. Schematic illustration of the quasiparticle excitation spectrum. The gapful spin excitations are separated from the gapless band of neutral singlet Majorana excitations by half the Brillouin zone.

where $\Delta_g\sim V^2/D$ and $m^*=(D/\Delta_g)m$ and m is the conduction-band mass at the band edge. Just above the gap, the quasiparticles have almost no conduction character: correlation functions of the local moments are then determined through the relation

$$\eta_j^b=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}\in 1/2\,\mathrm{BZ}}\{a_{\mathbf{k}b}e^{i\mathbf{k}\cdot\mathbf{R}_j}+a_{\mathbf{k}b}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{R}_j}\}\ . \tag{3.6}$$

(2) A neutral Majorana band, located around $\mathbf{k}=0$. These are the residual "scalar" excitations that do not condense into the odd-frequency paired state.

To gain more insight into these excitations, let us consider the conduction electron propagator

$$\mathcal{G}^{-1}(\omega)=[\omega-\tilde{\epsilon}_{\mathbf{k}}-\mu_{\mathbf{k}}\underline{\tau}_3-\underline{\Sigma(\kappa)}]\ . \tag{3.7}$$

We may align the spin reference frame axes to be parallel with the vectors $\hat{d}^{\lambda}$ by choosing

$$z_o=\begin{bmatrix}1\\0\end{bmatrix}\ , \tag{3.8}$$

so that $(\hat{d}^1,\hat{d}^2,\hat{d}^3)=(\hat{x},\hat{y},\hat{z})$, and $d_{ab}=\delta_{ab}$. With this choice of reference frame, then

$$\underline{\Sigma}(\kappa)=\frac{V^2}{\omega}\underline{\mathcal{P}},\quad \underline{\mathcal{P}}=\tfrac{1}{4}[3(\underline{1})-\sigma^a\otimes\tau^a]\ . \tag{3.9}$$

It is useful to define "up-" and "down-" spin projection operators:

$$\begin{aligned} P_{\uparrow}&=\tfrac{1}{2}[1+\sigma_3\otimes\tau_3]\ ,\\ P_{\downarrow}&=1-P_{\uparrow}=\tfrac{1}{2}[1-\sigma_3\otimes\tau_3]\ . \end{aligned} \tag{3.10}$$

We can use these operators to project out the "up" and "down" electron propagators ($G_\sigma P_\sigma=\mathcal{G}P_\sigma$):

$$\begin{aligned} G_{\uparrow}&=[(\omega-\tilde{\epsilon}_{\mathbf{k}}-\Delta_\omega)+\mu\tau_3+\Delta_\omega\tau_1]^{-1}\\ G_{\downarrow}&=[(\omega-\tilde{\epsilon}_{\mathbf{k}}-2\Delta_\omega)+\mu\tau_3]^{-1} \end{aligned}\qquad [\Delta_\omega=\Delta(\omega)]\ . \tag{3.11}$$

It is also useful to evaluate the determinants

$$\begin{aligned} \det[G_{\uparrow}^{-1}(\mathbf{k},\omega)]&=[(\omega-\tilde{\epsilon}_{\mathbf{k}}-\Delta_\omega)^2-\mu^2-\Delta_\omega^2]\ ,\\ \det[G_{\downarrow}^{-1}(\mathbf{k},\omega)]&=[(\omega-\tilde{\epsilon}_{\mathbf{k}}-2\Delta_\omega)^2-\mu^2]\ . \end{aligned} \tag{3.12}$$

Zeros of these functions determine the quasiparticle excitation energies $\omega_{\mathbf{k}\sigma}$ through $\det[G_\sigma^{-1}(\mathbf{k},\omega_{\mathbf{k}\sigma})]=0$ (Fig. 6).

The "down" propagator contains no pairing terms, and describes a gapful band of quasiparticles with excitation energies

$$\omega_{\mathbf{k}}=\frac{\tilde{\epsilon}_{\mathbf{k}}-\mu}{2}\pm\sqrt{[(\tilde{\epsilon}_{\mathbf{k}}-\mu)/2]^2+V^2}\ . \tag{3.13}$$

This spectrum closely resembles the large-N solution to the particle-hole symmetric Kondo model, with a hybridization gap $2\Delta_g$.[42–44]

The "up" electron propagator describes a band of odd-frequency paired electrons. The poles of this propagator

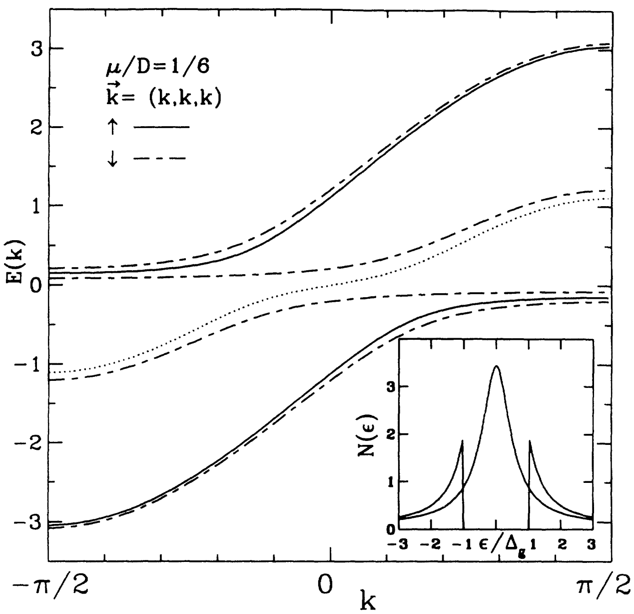


FIG. 6. Quasiparticle spectrum within mean-field theory for $\mu/D=\frac{1}{6}$. Bold line, gapped "up" excitations; dashed line, gapped "down" excitations; dotted line, neutral singlet Majorana band. Inset, density of states for up electron bands.

$$G_{\uparrow}(\omega)=\frac{(\omega-\tilde{\epsilon}_{\mathbf{k}}-\Delta_{\omega})-\mu\tau_3-\Delta_{\omega}\tau_1}{[(\omega-\tilde{\epsilon}_{\mathbf{k}}-\Delta_{\omega})^2-\mu^2-\Delta_{\omega}^2]} \tag{3.14}$$

at $\omega=\omega_{\mathbf{k}}$ are determined by the cubic equation $\det[G_{\uparrow}^{-1}(\mathbf{k},\omega_{\mathbf{k}})]=0$ [see Eq. (3.12)]. Solving for the conduction electron energy as a function of $\omega_{\mathbf{k}}$, $\epsilon_{\mathbf{k}}=\epsilon_{\pm}(\omega_k)$, we find

$$\epsilon_{\pm}(\omega_{\mathbf{k}})=[\omega_{\mathbf{k}}-\Delta(\omega_{\mathbf{k}})] \pm\operatorname{sgn}(\omega_{\mathbf{k}})\sqrt{[\Delta^2(\omega_{\mathbf{k}})+\mu^2]}\ , \tag{3.15}$$

which defines two branches of the "up" quasiparticle excitation spectrum. The $(-)$ branch is gapful with a gap $2\Delta_g\sim(2V^2/D)(1-\mu^2/D^2)^{-1}$, where D is the conduction electron half-bandwidth. The $(+)$ branch is gapless, corresponding to the Majorana component of the conduction sea that decouples from the resonant scattering center. The quasiparticle density of states corresponding to these two branches is

$$N^*_{\pm}(\omega)=\frac{\rho}{2}Z_{\pm}^{-1}(\omega)\ ,$$
$$Z_{\pm}^{-1}(\omega)=\frac{d\epsilon_{\pm}(\omega)}{d\omega}=\left\{1+\frac{\Delta_{\omega}}{\omega}\left[1\mp\frac{1}{\sqrt{1+(\mu/\Delta_{\omega})^2}}\right]\right\}. \tag{3.16}$$

At low energies

$$\omega_{\mathbf{k}(+)}=\epsilon_{\mathbf{k}}\left[1+\frac{\mu^2}{V^2}\right]^{-1} \tag{3.17}$$

giving an enhanced density of states $N^*_{+}(0)=\rho/2Z_O$, where $Z_O=[1+\mu^2/V^2]$, at the Fermi surface.

Let us explicitly construct these gapless quasiparticles. It is convenient to split the Hamiltonian into "up-" and "down-" spin parts $H=H_{\uparrow}+H_{\downarrow}$, where

$$H_{\downarrow}=\sum_{\mathbf{k}}\{(\epsilon_{\mathbf{k}}-\mu)\psi^{\dagger}_{\mathbf{k}\downarrow}\psi_{\mathbf{k}\downarrow}+V[\psi^{\dagger}_{\mathbf{k}\downarrow}\eta_{\mathbf{k}\downarrow}+(\mathrm{H.c.})]\}\ ,$$
$$\eta_{\mathbf{k}\downarrow}=\frac{1}{\sqrt{2}}[\eta^1_{\mathbf{k}}+i\eta^2_{\mathbf{k}}]\ , \tag{3.18}$$

describes the hybridized band of unpaired "down" electrons, and

$$H_{\uparrow}=\sum_{\mathbf{k}\in\frac{1}{2}\mathrm{BZ}}A^{\dagger}_{\mathbf{k}}\underline{h}_{\mathbf{k}}A_{\mathbf{k}}\ ,$$
$$\underline{h}_{\mathbf{k}}=\left[\begin{array}{c|c}\epsilon_{\mathbf{k}}\underline{1}-\mu\underline{\tau_3} & \begin{array}{c}\frac{V}{\sqrt{2}}\\ -\frac{V}{\sqrt{2}}\end{array}\\ \hline \frac{V}{\sqrt{2}}\ -\frac{V}{\sqrt{2}} & 0\end{array}\right]\ , \tag{3.19}$$
$$A^{\dagger}_{\mathbf{k}}=(\psi^{\dagger}_{\mathbf{k}\uparrow},\psi_{-\mathbf{k}\uparrow},\eta^{3\dagger}_{\mathbf{k}})\ ,$$

describes the paired "up" electrons. In terms of the quasiparticle operators

$$H_{\uparrow}=\sum_{\mathbf{k}}\omega_{\mathbf{k}\alpha}a^{\dagger}_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}\ , \tag{3.20}$$

where only positive energies enter into the Hamiltonian. Here $\alpha=0,3$ denotes the gapless and gapful excitation branch, respectively. The quasiparticle operators for the gapless "up" electrons can be constructed from a generalized Bogoliubov transformation

$$a^{\dagger}_{\mathbf{k}0}=\sqrt{Z_{\mathbf{k}}}(u_{\mathbf{k}}\psi^{\dagger}_{\mathbf{k}\uparrow}+v_{\mathbf{k}}\psi_{-\mathbf{k}\uparrow})+\sqrt{(1-Z_{\mathbf{k}})}\eta^{3\dagger}_{\mathbf{k}}\ . \tag{3.21}$$

The eigenvector $\phi_{\mathbf{k}}$ containing the Bogoliubov coefficients satisfies

$$\underline{h}_{\mathbf{k}}\phi_{\mathbf{k}}=\omega_{\mathbf{k}0}\phi_{\mathbf{k}}\ . \tag{3.22}$$

Eliminating $Z_{\mathbf{k}}$ and substituting back into Eq. (3.22) then gives

$$\underline{G}_{\uparrow}^{-1}(\mathbf{k},\omega_{\mathbf{k}})\begin{bmatrix}u_{\mathbf{k}}\\ v_{\mathbf{k}}\end{bmatrix}=0\ , \tag{3.23}$$

where $\underline{G}_{\uparrow}^{-1}(\kappa)$ is taken from Eq. (3.11). Diagonalizing this eigenvalue equation gives $u_{\mathbf{k}}=u^2(\omega_{\mathbf{k}0})$, $v_{\mathbf{k}}=v^2(\omega_{\mathbf{k}0})$, where

$$u^2(\omega)=\frac{1}{2}\left[1+\frac{\mu}{\sqrt{\Delta_{\omega}^2+\mu^2}}\right]\ ,$$
$$v^2(\omega)=\frac{1}{2}\left[1-\frac{\mu}{\sqrt{\Delta_{\omega}^2+\mu^2}}\right]\ , \tag{3.24}$$

where the energies are given by Eq. (3.15). $Z_{\mathbf{k}}=Z_{+}(\omega_{\mathbf{k}+})$ takes the form given in Eq. (3.16). Energy, rather than momentum-dependent Bogoliubov coefficients, is a characteristic of odd-frequency pairing.

Let us now consider the charge and spin coherence factors of these gapless excitations. In BCS superconductors, the Bogoliubov quasiparticles contain an equal weight of "electron" and "hole" at the gap energy, which leads to a vanishing of the charge coherence factor. A similar phenomenon occurs in odd-frequency pairing, but in this case it occurs at zero energy. We see from the discussion above that at the Fermi energy $u(0)=v(0)=1/\sqrt{2}$, and so the gapless quasiparticles are a precise linear combination of "up electron" and "down hole:"

$$a^{\dagger}_{\mathbf{k}_F 0}=\sqrt{Z_O/2}(\psi^{\dagger}_{\mathbf{k}_F\uparrow}+\psi_{-\mathbf{k}_F\uparrow})+\sqrt{(1-Z_O)}\eta^{3\dagger}_{\mathbf{k}} . \quad (3.25)$$

The equal weight of particles with opposite spin and charge quantum numbers implies that the spin and charge coherence factors will vanish at low energies, leading to neutral, spinless excitations.

To see this in detail, note first that within the gapless "up" band only the conduction charge and spin operators contain diagonal matrix elements. Suppose we attempt to excite quasiparticles out of the ground state by coupling to a charge or spin excitation; the relevant diagonal matrix elements are then

$$\left\langle \mathbf{k}^- \left| \begin{Bmatrix} \rho_{\mathbf{q}} \\ \sigma^z_{\mathbf{q}} \end{Bmatrix} \right| \mathbf{k}^+ \right\rangle = \langle \mathbf{k}^- | \{ \psi^{\dagger}_{\mathbf{k}^-\uparrow}\psi_{\mathbf{k}^+\uparrow} - \psi_{-\mathbf{k}^-\uparrow}\psi^{\dagger}_{-\mathbf{k}^+\uparrow} \} | \mathbf{k}^+ \rangle , \quad (3.26)$$

where $\mathbf{k}^{\pm}=\mathbf{k}\pm\mathbf{q}/2$ and $|\mathbf{k}^{\pm}\rangle=a^{\dagger}_{\mathbf{k}^{\pm}}|0\rangle$ denotes the state with one quasiparticle added to the mean-field ground state. In terms of the Bogoliubov coefficients this is

$$\left\langle \mathbf{k}^- \left| \begin{Bmatrix} \rho_{\mathbf{q}} \\ \sigma^z_{\mathbf{q}} \end{Bmatrix} \right| \mathbf{k}^+ \right\rangle = \sqrt{Z_{\mathbf{k}^+}Z_{\mathbf{k}^-}}[u_+u_- - v_+v_-] , \quad (3.27)$$

where $u_{\pm}=u(\omega_{\mathbf{k}^{\pm}})$ and $v_{\pm}=v(\omega_{\mathbf{k}^{\pm}})$ are the Bogoliubov factors in the gapless band (+). On the Fermi surface, since $u=v=1/\sqrt{2}$, this coherence factor *vanishes.* Away from the Fermi surface, the spin-charge coherence factor grows linearly with energy

$$\left\langle \mathbf{k}^- \left| \begin{Bmatrix} \rho_{\mathbf{q}} \\ \sigma^z_{\mathbf{q}} \end{Bmatrix} \right| \mathbf{k}^+ \right\rangle = (\omega_{\mathbf{k}^+}+\omega_{\mathbf{k}^-}) \left[\frac{\mu}{V^2+\mu^2} \right] \quad (\omega_+,\omega_- \ll \Delta_g) . \quad (3.28)$$

(In the special case of particle-hole symmetry, these coherence factors vanish *throughout* the gap.) In a similar fashion, we may examine quasiparticle components of the charge and spin given by

$$\begin{Bmatrix} Q \\ \sigma^z \end{Bmatrix}_{\mathbf{k}} = \lim_{\mathbf{q}\to 0} \left\langle \mathbf{k}^- \left| \begin{Bmatrix} \rho_{\mathbf{q}} \\ \sigma^z_{\mathbf{q}} \end{Bmatrix} \right| \mathbf{k}^+ \right\rangle = Z_{\mathbf{k}}[u^2_{\mathbf{k}}-v^2_{\mathbf{k}}] = Z(\omega_{\mathbf{k}})\frac{\mu}{\sqrt{\Delta^2(\omega_{\mathbf{k}})+\mu^2}} \sim \frac{2\mu\omega_{\mathbf{k}}}{\mu^2+V^2} \quad (\omega_{\mathbf{k}} \ll \Delta_g) . \quad (3.29)$$

From these results, we conclude that there is no way to couple via charge or spin probes to the quasiparticle excitations at the Fermi surface. These gapless excitations are devoid of charge or spin quantum numbers on the Fermi surface. This dramatic effect is a direct consequence of the resonant pairing and the pole in the gap function. So long as this pole is maintained, the coherence factors will identically vanish on the Fermi surface. Note, however, that these quasiparticles can still carry entropy, and in this sense can be regarded as thermal quasiparticles.

It is particularly instructive to examine the *local* conduction electron propagator and the pair wave function in this simple mean-field theory. The local propagator for the paired "up" electrons is

$$\underline{G}_{\uparrow}(\omega)=\sum_{\mathbf{k}}\underline{G}_{\uparrow}(\mathbf{k},\omega)=\rho\int_{-D}^{D}d\epsilon\, G_{\uparrow}(\epsilon,\omega) . \quad (3.30)$$

Carrying out the integral over the conduction electron energies we find

$$\frac{1}{\pi\rho}\mathrm{Im}[\underline{G}_{\uparrow}(\omega-i\delta)] = \begin{cases} \underline{1} \quad (|\omega|>\Delta_g) , \\ \dfrac{1}{2}\left[1+\mathrm{sgn}(\omega)\dfrac{\Delta(\omega)\tau_1+\mu\tau_3}{\sqrt{\Delta(\omega)^2+\mu^2}} \right] \quad (|\omega|<\Delta_g) . \end{cases} \quad (3.31)$$

Loosely speaking, the electrons are normal outside the gap region and become paired at energies less than the gap Δ_g. The spectral function can be rewritten in terms of the energy-dependent Bogoliubov coefficients derived in Eq. (3.24):

$$\frac{1}{\pi\rho}\mathrm{Im}[\underline{G}_{\uparrow}(\omega-i\delta)] = \begin{bmatrix} u^2_{\omega} & u_{\omega}v_{\omega} \\ u_{\omega}v_{\omega} & v^2_{\omega} \end{bmatrix} , \quad (3.32)$$

where the coefficients u_{ω} and v_{ω} are evaluated in the gapless band.

Finally, we may construct the pair wave function from the off-diagonal components of this spectral function

$$\langle \psi_\uparrow(x,i\omega_n)\psi_\uparrow(x,-i\omega_n)\rangle = \frac{\rho}{2}\int_{-D}^{D}\frac{d\omega}{\pi}\frac{1}{i\omega_n-\omega}\frac{\Delta(\omega)\mathrm{sgn}(\omega)}{\sqrt{\Delta(\omega)^2+\mu^2}}$$
$$= -i\omega_n\rho\int_0^D\frac{d\omega}{\pi}\frac{1}{[\omega_n^2+\omega^2]}\frac{\Delta(\omega)}{\sqrt{\Delta(\omega)^2+\mu^2}}\ , \qquad (3.33)$$

thereby explicitly displaying the odd-frequency character of the pairing.

IV. MEAN-FIELD THERMODYNAMICS

Next we discuss the mean-field thermodynamics. The mean-field free energy per site is written in terms of the conduction electron propagators as

$$F_{\mathrm{MF}} = \frac{V^2}{J} - \frac{T}{2}\sum_\kappa \mathrm{Tr}\ln[\mathcal{G}^{-1}(\kappa)]$$
$$= \frac{V^2}{J} - \frac{T}{2}\sum_\kappa \ln\{\det[\mathcal{G}^{-1}(\kappa)]\}\ , \qquad (4.1)$$

where the determinant can be expanded in terms of the "up" and "down" components of the propagator [Eq. (3.11)]:

$$\det[\mathcal{G}^{-1}(\kappa)] = \det[G_\uparrow^{-1}(\kappa)]\det[G_\downarrow^{-1}(\kappa)]\ . \qquad (4.2)$$

Differentiating with respect to the order parameter yields the mean-field equation

$$\frac{1}{J}+\frac{T}{2}\sum_\kappa\frac{1}{i\omega_n}\left\{\frac{i\omega_n-\tilde{\epsilon}_{\mathbf{k}}}{\det[G_\uparrow^{-1}(\kappa)]}+\frac{2(i\omega_n-\tilde{\epsilon}_{\mathbf{k}}-2\Delta_n)}{\det[G_\downarrow^{-1}(\kappa)]}\right\}=0\ , \qquad (4.3)$$

where the denominators in these equations are given in Eq. (3.12). For a constant conduction electron density of states ρ, we may replace

$$\sum_{\mathbf{k}}\{\cdots\}\to\rho\int_{-D}^{D}d\epsilon\{\cdots\}=\rho\int\frac{dz}{2\pi i}\Theta[z]\{\cdots\}\ , \qquad (4.4)$$

where the contour integral proceeds clockwise around the branch cut in the function

$$\Theta[z]=\ln\left[\frac{z-D}{-D-z}\right]\ . \qquad (4.5)$$

The energy integrals can then be performed by closing the contour around the poles in the Green's functions, which are located at

$$\epsilon_{\uparrow\alpha}(\omega)=\omega-\Delta_\omega+\alpha\,\mathrm{sgn}(\omega)\sqrt{\Delta_\omega^2+\mu^2}$$
$$\epsilon_{\downarrow\alpha}(\omega)=\omega-2\Delta_\omega+\alpha\mu \qquad (\alpha=\pm) \qquad (4.6)$$

for the up and down electrons, respectively. Carrying out the complex integral then gives

$$\frac{1}{J}=\frac{\pi T}{2}\sum_{\substack{i\omega_n\\ \alpha=\pm}}\frac{1}{i\omega_n}\left\{F_{\uparrow\alpha}(i\omega_n)\left[\frac{1}{2}-\frac{\alpha\Delta_n}{2\sqrt{(\Delta_n^2+\mu^2)}}\right]+F_{\downarrow\alpha}(i\omega_n)\right\}\ , \qquad (4.7)$$

where $F_{\sigma\alpha}(z)=\rho\Theta[\epsilon_{\sigma\alpha}(z)]/\pi$ and we have used the notation $\Delta_n\equiv\Delta(i\omega_n)$. Carrying out the Matsubara sums then yields

$$\frac{1}{J}=\sum_{\alpha=\pm}\int\frac{d\omega}{4\omega}\mathrm{th}\left[\frac{\beta\omega}{2}\right]\left\{\frac{F''_{\uparrow\alpha}(\omega^+)}{2}\left[1-\frac{\alpha|\Delta_\omega|}{\sqrt{(\Delta_\omega^2+\mu^2)}}\right]+F''_{\downarrow\alpha}(\omega^+)\right\}\ , \qquad (4.8)$$

where $\omega^+=\omega+i\delta$. The functions $F''_{\sigma\alpha}(\omega^+)\equiv\mathrm{Im}F_{\sigma\alpha}(\omega^+)$ count the number of up and down excitation branches at frequency ω. Ignoring the small differences between the up- and down-spin excitation gaps,

$$F''_{\sigma\alpha}(\omega^+)=\rho\begin{cases}\theta(D-|\omega|) & (\sigma=\uparrow\alpha=+)\ ,\\ \theta(D-|\omega|)-\theta(\Delta_g-|\omega|) & (\text{otherwise})\ ,\end{cases} \qquad (4.9)$$

for the gapless and gapful branches, respectively. This simple mean-field theory then gives rise to a phase transition at a temperature

$$T_c\sim D\exp\left[-\frac{1}{3/2J\rho}\right]=T_K\exp\left[-\frac{1}{6J\rho}\right]\ , \qquad (4.10)$$

where $T_K=D\exp[-1/(2J\rho)]$ is the single-ion Kondo temperature. At $\mu=0$, the gapless excitation branch of the spectrum does not contribute to the mean-field equation. At finite μ, the gapless branch develops a small linear coherence factor, and we see that this has the effect of suppressing the transition temperature. For all values of μ, however, the form of the mean-field $\Delta_g(T)$ quite closely resembles that of a singlet BCS superconductor.

It is clear that there are several weaknesses to the theory from these results. First, note that the mean-field transition occurs from a state where the local moments are unquenched, directly into a heavy-fermion superconductor, without any intermediate heavy Fermi-liquid phase. Though we presume that key aspects of the heavy-fermion phase might be recovered by including the self-energy effects of fluctuations on the conduction electrons, this has yet to be established. The precise relation between the single-ion Kondo temperature and T_c is also not reliably predicted by the mean-field theory. Our path-integral approach amounts to a "Hartree" decoupling of the interaction. Had we chosen a more conventional diagrammatic approach, carrying out a "Hartree-Fock" decoupling of the original Hamiltonian, writing

$$\langle \eta\psi_j \rangle = \overline{\eta\psi}_j = -\frac{1}{2J}\sigma \begin{bmatrix} V_{j\uparrow} \\ V_{j\downarrow} \end{bmatrix} \tag{4.11}$$

so that

$$-i\frac{J}{2}\overline{\psi_j^\dagger \eta}\times\overline{\eta\cdot\sigma\psi_j} - i\frac{J}{2}\overline{\psi_j^\dagger \underline{\eta\times\eta\cdot\sigma}\psi_j} \rightarrow -\frac{3}{2J}V_j^\dagger V_j \tag{4.12}$$

then the mean-field Hamiltonian would have become

$$H_{\text{int}}[j] = \rightarrow \psi_j^\dagger(\sigma\cdot\eta_j)V_j + V_j^\dagger(\sigma\cdot\eta_j)\psi_j + 3|V_j|^2/2J \tag{4.13}$$

so that for this scheme, $T_c^{\text{MF}} = T_K$, to logarithmic accuracy. The path-integral approach recovers the "Fock" contributions to the pairing as a leading-order component of the random-phase-approximation (RPA) fluctuation corrections to the mean-field transition temperature (Fig. 7). Since fluctuation effects will suppress T_c in either scheme, the particular choice of mean-field theory is somewhat arbitrary, and will not matter at the next level of approximation.

If we take our mean-field theory literally, we see that from the point of view of the original conduction band, the transition into the odd-frequency state can occur for an arbitrarily weak-coupling constant, taking advantage of the Kondo effect to produce a logarithmic divergence in the pairing channel. Past treatment of odd-frequency pairing required a finite coupling constant: here, the $1/\omega$ divergence in the gap function provides an infinitely strong pairing field that moves the critical coupling to zero again. Significant pair breaking effects will, of course, come from the fluctuations. In the one-impurity problem, there are infrared divergences in the Gaussian fluctuations that suppress the mean-field transition temperature to zero. However (unlike the large-N approach), in the lattice model there is *no* continuous gauge symmetry so the development of a gap in the spectrum will cut off the one-impurity infrared divergences, preserving a finite-temperature transition.

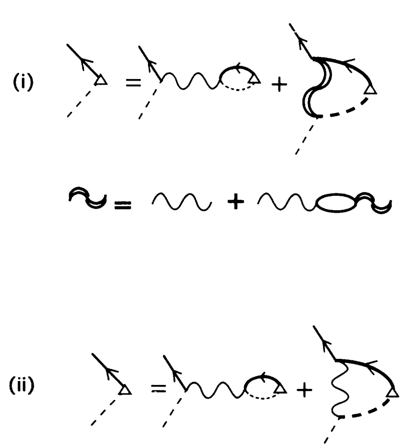


FIG. 7. Illustrating the distinction between (i) the Hartree/RPA decoupling scheme used and (ii) a Hartree-Fock decoupling procedure. The "Fock" part of the vertex equation is absent from the Hartree approximation, but is reincorporated as a leading term in the RPA.

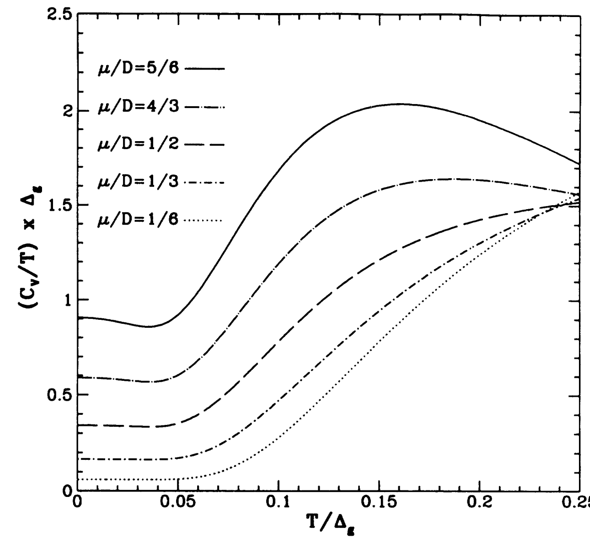


FIG. 8. Temperature dependence of the specific heat, calculated at low temperatures for a variety of μ/D. Note that as μ/D increases, the gapless band becomes "heavy."

Finally, we note that expanding the free energy at low temperatures yields a linear specific heat proportional to the density of states in the gapless band:

$$\begin{aligned}\gamma &= \frac{\pi^2 k_B^2}{3}\frac{\rho}{2}\left[1+\left[\frac{\mu}{V}\right]^2\right] \\ &= \frac{\pi^2 k_B^2}{3}\frac{1}{2}\left[\rho+\frac{1}{2\Delta_g}\left[\frac{\mu}{D}\right]^2\right] .\end{aligned} \tag{4.14}$$

Depending on the ratio (μ/D), this linear specific heat can range from a value characteristic of the free conduction band, $(\mu/D)\sim 0$, to a value more characteristic of a heavy-fermion metal $\sim 1/\Delta_g$ for $(\mu/D)\sim 1$ (Fig. 8). The quantity $(\mu/D)^2$ is a measure of the particle-hole asymmetry. In a more realistic band structure, this quantity is replaced by the average of the particle-hole asymmetry over the Brillouin zone

$$\left[\frac{\mu}{D}\right]^2 \rightarrow \left\langle \left[\frac{\mu_{\mathbf{k}}}{D}\right]^2 \right\rangle_{\mathbf{k}} . \tag{4.15}$$

In general, this ratio can be significant even when close to half filling.

V. RIGIDITY OF THE ODD-FREQUENCY PAIRED STATE

One of the key issues associated with odd frequency pairing, is whether it leads to a real superconducting Meissner effect. Past attempts to construct an odd-frequency paired state within an Eliashberg formalism have experienced difficulty in producing a state with a positive phase stiffness[45] and a finite London penetration depth. To begin our discussion, we first discuss the form of the long-wavelength effective action.

A. Long-wavelength action

In general, the mean-field free energy will depend on gradients of the order-parameter field, and the form of the applied vector potential. Let us now consider slow deformations of the order parameter

$$z(x)=g(x)\begin{bmatrix}1\\0\end{bmatrix}, \tag{5.1}$$

where

$$g(x)=e^{[i\theta(x)\cdot\mathbf{s}]}=\begin{bmatrix}z_\uparrow & -z_\downarrow^*\\ z_\downarrow & z_\uparrow^*\end{bmatrix},\quad \mathbf{s}=\left[\frac{\sigma}{2}\right] \tag{5.2}$$

is an SU(2) rotation matrix. The rate of rotation is given by $\nabla g=g\omega$, where

$$\omega=g^{-1}\nabla g=i\omega_\lambda s^\lambda \tag{5.3}$$

is decomposed in terms of its components $\omega_\lambda(x)$ along the principal axes $\hat{d}_\lambda$ of the order parameter. The leading quadratic terms in the gradient expansion of the free energy about the uniform mean-field theory are then

$$F=\sum_{\lambda=1,3}\frac{\rho_\lambda}{2}\int \omega_\lambda^2 d^3x\ . \tag{5.4}$$

Here the stiffnesses ρ_λ for slow twists about each principal axis are analogous to the moments of inertia of a top.

To include the effects of an external magnetic field, we introduce a finite vector potential by an appeal to gauge invariance. Our original model is gauge invariant under the transformation

$$\begin{aligned}&\psi(x)\to e^{i\phi(x)}\psi(x)\ ,\\ &z(x)\to e^{i\phi(x)}z(x)\ ,\\ &\mathbf{A}(x)\to \mathbf{A}(x)+\left[\frac{\hbar}{e}\right]\nabla\phi(x)\ ,\end{aligned} \tag{5.5}$$

so that

$$g(x)\to g(x)e^{i\phi(x)\sigma_3}\ . \tag{5.6}$$

This means that the long-wavelength action must be invariant under the transformation

$$\begin{aligned}&\omega_3\to\omega_3+2\nabla\phi(x)\ ,\\ &\frac{e}{\hbar}\mathbf{A}(x)\to\frac{e}{\hbar}\mathbf{A}(x)+\nabla\phi(x)\ .\end{aligned} \tag{5.7}$$

In other words, a uniform vector potential $\mathbf{A}$ is equivalent to a uniform rotation rate $-(2e/\hbar)\mathbf{A}$ about the $\hat{d}_3$ axis. That rotations about the $\hat{d}_3$ axis are equivalent to gauge transformations can be understood by noting that multiplication of a unit spinor by a phase factor $e^{i\phi}$ is equivalent to rotating its principal axes through an angle 2ϕ:

$$\begin{bmatrix}1\\0\end{bmatrix}\to e^{i\phi}\begin{bmatrix}1\\0\end{bmatrix}\equiv e^{i2\phi(\sigma^z/2)}\begin{bmatrix}1\\0\end{bmatrix}\ . \tag{5.8}$$

The gauge-invariant form of the free energy is then

$$F=\frac{1}{2}\int d^3x\left[\rho_m\omega_\perp^2+\rho_s\left[\omega_3-\frac{2e}{\hbar}\mathbf{A}\right]^2+\frac{B^2}{\mu_o}\right]\ . \tag{5.9}$$

In terms of the vector $\hat{n}\equiv\hat{d}_3=z^\dagger\sigma z$, this action can also be written

$$F=\frac{1}{2}\int d^3x\left[\rho_m(\nabla\hat{n})^2+\rho_s\left[\omega_3-\frac{2e}{\hbar}\mathbf{A}\right]^2+\frac{B^2}{\mu_o}\right]\ . \tag{5.10}$$

The term ρ_s is the Meissner stiffness of the superconductor, whereas the term ρ_m can be regarded as a "spin stiffness" of the triplet paired state. It is at first surprising that a charge $1e$ spinor order parameter can give rise to a charge $2e$ coupling between gradients of the phase and the vector potential. We can resolve this apparent paradox by noting that $z(x)$ is also a spin-$\frac{1}{2}$ object, thus a change in phase of $z(x)$ of ϕ corresponds to a rotation through an angle $\theta=2\pi$. A rotation of the physical order parameter through 2π corresponds to a sign change in $z(x)\to -z(x)$ and so $z(x)$ must be continuous up to a sign ±1. The gauge-invariant coupling between ϕ and $\mathbf{A}$ is then

$$\left[\nabla\phi-\frac{e}{\hbar}\mathbf{A}\right]^2\to\frac{1}{4}\left[\nabla\theta-\frac{2e}{\hbar}\mathbf{A}\right]^2 \tag{5.11}$$

and hence the coupling between physical rotations and the vector potential is a charge $2e$ coupling, as in conventional superconductivity. Note finally that if we include spin anisotropy into the original Hamiltonian, then this will tend to align the order parameter, for example, through the inclusion of a term of the form

$$F_a=-\frac{\rho_m}{l_o^2}\int d^3x(\hat{d}_3\cdot\hat{z})^2\ . \tag{5.12}$$

On length scales $l>l_o$, the system behaves as a conventional Landau-Ginzburg theory.

B. Computation of the Meissner stiffness

To compute the Meissner and spin stiffnesses in this gradient expansion, we consider a configuration with a uniform rotation about the principal axes $\hat{d}_a$

$$z_j=e^{[i\omega\cdot\mathbf{R}_jS^a]}z_j^0\quad\left[S^a\equiv\frac{\sigma^a}{2}\right]\ . \tag{5.13}$$

We may absorb this uniform rotation into a gauge transformation of the conduction electrons through the replacement of the conduction electron kinetic energy by

$$\begin{aligned}&\epsilon_{\mathbf{k}}\to\epsilon_{\mathbf{k}-\omega S^a}=\epsilon_{\mathbf{k}}+h(\mathbf{k})\ ,\\ &\underline{h}(\mathbf{k})=-\omega_\mu\nabla_\mu\epsilon_{\mathbf{k}}\underline{S}^a+\tfrac{1}{8}\omega_\mu\omega_\nu\nabla^2_{\mu\nu}\epsilon_{\mathbf{k}}\ .\end{aligned} \tag{5.14}$$

Here we have expanded the kinetic energy to quadratic order in the twist. The effect of the twist in the phase can then be included into the electronic Green's function by

$$-\mathcal{G}^{-1}(\kappa)\to-\mathcal{G}^{-1}(\kappa)+h(\kappa)\ . \tag{5.15}$$

The free energy of the system in the presence of a uniform twist can be calculated from the trace of the conduction electron propagator as follows:

$$\begin{aligned}F[\omega_a]-F[0]&=-\frac{T}{2}\sum_{\kappa}\mathrm{Tr}\{\ln[-\mathcal{G}^{-1}(\kappa)+h(\kappa)]\\&\qquad-\ln[-\mathcal{G}^{-1}(\kappa)]\}\\&=-\frac{T}{2}\sum_{\kappa}\mathrm{Tr}\{\ln[1-\mathcal{G}(\kappa)h(\kappa)]\}\ .\end{aligned} \tag{5.16}$$

Expanding the logarithm to quadratic order gives

$$\begin{aligned}&F[\omega]-F[0]=\frac{\rho_a\omega^2}{2}\ ,\\&\rho^a=\frac{T}{8}\sum_{\kappa}\left[\frac{\nabla^2\tilde{\epsilon}_{\mathbf{k}}}{3}\right]\mathrm{Tr}[\mathcal{G}(\kappa)]+\nabla\tilde{\epsilon}_{\mathbf{k}}^2\mathrm{Tr}[\mathcal{G}(\kappa)\sigma^a\mathcal{G}(\kappa)\sigma^a]\ .\end{aligned} \tag{5.17}$$

The first term in ρ^a can be integrated by parts to yield

$$\rho^a=\frac{T}{8}\sum_{\kappa}(\nabla\tilde{\epsilon}_{\mathbf{k}})^2\mathrm{Tr}[\mathcal{G}(\kappa)\sigma^a\mathcal{G}(\kappa)\sigma^a-\mathcal{G}(\kappa)^2] \tag{5.18}$$

for the stiffness about the $\mathbf{d}_a$ axis. For our simple model, $\rho^1=\rho^2=\rho_m$, and in the special case where $\mu=0$ all three stiffnesses are equal. We shall explicitly focus on the stiffness about the $\hat{n}\equiv\hat{d}_3$ axis, which is associated with the London kernel

$$\begin{aligned}&\frac{\partial^2F}{\partial A_\nu\partial A_\mu}=Q_{\mu\nu}\ ,\\&Q_{\mu\nu}=4e^2\rho_3\delta_{\mu\nu}\ .\end{aligned} \tag{5.19}$$

We can separate the trace into "up" and "down" components. The "down" component is unpaired and explicitly vanishes. The "up" component gives

$$\rho_3=-\frac{T}{4}\sum_{\kappa}\mathbf{v}_{\mathbf{k}}^2\frac{2\Delta_n^2}{[(i\omega_n-\Delta_n-\tilde{\epsilon}_{\mathbf{k}})^2-\Delta_n^2-\mu^2]^2}\qquad(\mathbf{v}_{\mathbf{k}}=\nabla\tilde{\epsilon}_{\mathbf{k}})\ . \tag{5.20}$$

In a conventional BCS theory, it is sufficient to impose a low-energy cutoff on the frequency sum,

$$|\omega_n|\le\Lambda\ , \tag{5.21}$$

after which the conduction electron bandwidth can be taken to infinity. We are unable to take this continuum limit, for we must maintain the value of the excitation gap of the unpaired down electrons $\Delta_g\sim V^2/D$: this means that we must maintain a finite band electron cutoff. [In other words, the number of electrons per local moment $\sim N(0)D$ must remain finite.] Since our mean-field theory will not be accurate at frequency scales that are large compared with the Kondo temperature, we shall choose a frequency cutoff that is intermediate between the conduction electron bandwidth and the Kondo temperature

$$T_K\ll\Lambda\ll D\ . \tag{5.22}$$

With this choice, we are able to replace the density of states by its value at the Fermi surface: the energy integral is then carried out in the same fashion as Sec. IV, replacing

$$\sum_{\mathbf{k}}\{\cdots\}\to\rho\int_{-D}^{D}d\epsilon\{\cdots\}=\rho\int\frac{dz}{2\pi i}\Theta[z]\{\cdots\}\ , \tag{5.23}$$

where the contour integral proceeds clockwise around the branch cut in the function $\Theta[z]=\ln[(z-D)/(-D-z)]$. The frequency sums can then be performed by closing the contour around the poles in the Green's functions, which are located at

$$\epsilon_{\uparrow\alpha}(\omega)=\omega-\Delta_\omega+\alpha\,\mathrm{sgn}(\omega)\sqrt{\Delta_\omega^2+\mu^2}\quad(\alpha=\pm)\ . \tag{5.24}$$

Carrying out the contour integral in $z=\epsilon$ then gives

$$\begin{aligned}\rho_3&=\frac{\rho v_F^2T}{24}\sum_{i\omega_n,\alpha}\frac{\alpha\Delta_n^2}{(\Delta_n^2+\mu^2)^{3/2}}\Theta[\epsilon_\alpha(i\omega_n)]\\&=\frac{\rho v_F^2}{24}\sum_{\alpha}\int\frac{d\omega}{2\pi}\mathrm{Im}\{\Theta[\epsilon_\alpha(\omega+i\delta)]\}\mathrm{th}[\beta\omega/2]\\&\qquad\times\frac{\alpha\Delta_\omega^2}{(\Delta_\omega^2+\mu^2)^{3/2}}\ .\end{aligned} \tag{5.25}$$

These two poles cancel one another's contributions, except in the gap region $|\omega|<\Delta_g$, where the gapless excitation branch contributes a finite amount to the stiffness. Our final result for the London stiffness is then

$$Q=4e^2\rho_3=\frac{Ne^2}{4m}\int_0^{\Delta_g}d\omega\,\mathrm{th}\left[\frac{\beta\omega}{2}\right]\frac{\Delta_\omega^2}{(\Delta_\omega^2+\mu^2)^{3/2}}\left[\Delta_\omega=\frac{V^2}{2\omega}\right]\ , \tag{5.26}$$

where we have set $N/m\equiv2\rho v_F^2/3$. By making the low-temperature expansion

$$\mathrm{th}\left[\frac{\beta\omega}{2}\right]=\mathrm{sgn}(\omega)+\frac{\pi^2T^2}{3}\delta'(\omega)+O(T^4)\ , \tag{5.27}$$

the temperature dependence of the Meissner stiffness and penetration depth become

$$\frac{1}{\lambda_L^2(T)}=\frac{1}{(\lambda_L^o)^2}\left[1-F\left[\frac{\mu}{D}\right]\frac{\pi^2T^2}{3\Delta_g^2}\right]\ , \tag{5.28}$$

where $4\pi Q(T)=[\lambda_L(T)]^{-2}$ defines the London penetration depth and

$$F(x)=2x^2\left[1-\frac{1}{\sqrt{1+4x^2}}\right]^{-1}\ . \tag{5.29}$$

This T^2 variation of the penetration depth is similar to that expected for point nodes in a conventional pairing scenario. In the special case of $\mu=0$, the Meissner stiffness is simply

$$Q=\frac{Ne^2}{m}\left[\frac{\Delta_g^2}{4V^2}\right]\approx\frac{Ne^2}{m}\left[\frac{\Delta_g}{4D}\right], \quad (5.30)$$

where we have set $\Delta_g=V^2/D$. The stiffness of the order parameter is thus finite, but suppressed by a factor of $Z=\Delta_g/D$ compared with a conventional metal. Loosely speaking, we may consider this to be an effect of the condensation of heavy fermions, whose effective mass is enhanced by a factor $m^*/m\sim 1/Z$, and whose rigidity is then depressed by the factor $m/m^*\sim Z$.

The staggered phase of the order parameter plays a critical role in developing this finite stiffness. This point is illustrated in Fig. 9. The "uniform" odd-frequency triplet state ($\mathbf{Q}=0$) is unstable and its energy may be monotonically reduced by twisting the order parameter until the stable minimum at $\mathbf{Q}=(\pi,\pi,\pi)$ is reached.

The "spin stiffness" $\rho_m=\rho_{1,2}$ for twisting the order parameter about the $\hat{d}_\perp$ axes can be calculated in a similar fashion. When $\mu=0$, the system is particle-hole symmetric, and $\rho_m=\rho_3$ as given above. Like the superfluid stiffness ρ_s, contributions to the stiffness come predominantly from the neutral excitation band inside the gap, though the formal expression for $\mu\neq 0$ is more complicated, and shall not be given here.

C. Collective modes

To end our discussion on the long-wavelength properties, we should like to briefly mention the collective modes of the condensate. Let us generalize the effective action to incorporate the leading-order time dependence of the pairing field

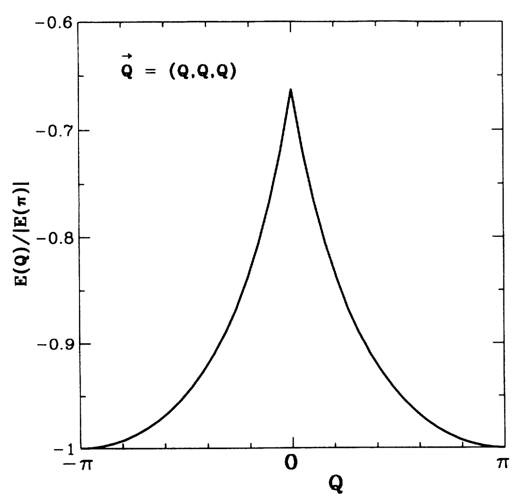


FIG. 9. Mean-field free energy of the odd-frequency paired state plotted as a function of the "twist" wave vector of the triplet pairing field $\hat{d}_c(\mathbf{R})=e^{i\mathbf{Q}\cdot\mathbf{R}}\hat{d}_c(0)$. The uniform state ($Q=0$) is unstable with respect to the state with a staggered phase ($Q=\pi$).

$$S=\frac{1}{2}\int dt\, d^3x\left[\{\chi_m(\partial_t\hat{n})^2-\rho_m(\nabla\hat{n})^2\}+\left\{\chi\left[\omega_3^0-\frac{2e}{\hbar}V\right]^2-\rho_s\left[\omega_3-\frac{2e}{\hbar}\mathbf{A}\right]^2\right\}+\left[\frac{(E/c)^2-B^2}{\mu_o}\right]\right], \quad (5.31)$$

where χ_m denotes the magnetic or spin susceptibility and χ denotes the charge susceptibility. An applied vector potential is gauge equivalent to a rotation about the $\hat{d}^3$ axis, and must be included with the kinetic terms to maintain the gauge invariance, as explained above. The spin and charge susceptibilities are given by $\chi=\chi_m=\rho$. In the absence of a coupling to the electromagnetic field, this action would give rise to a collective phase mode, and a spin-wave mode, with velocities

$$v_{\text{spin}}^2\sim v_{\text{phase}}^2\sim v_F^2\left[\frac{T_K}{D}\right]. \quad (5.32)$$

Of course, phase modes are gauged away as fluctuations of the electromagnetic field, converting the phase mode into a longitudinal plasmon mode as part of the Meissner effect, following the well-known Anderson-Higgs mechanism.[46] The spin-wave mode cannot be gauged away in this fashion and is *unscreened,* leading to gapless collective spin modes in the superconducting state that coexist with the superconductivity. From the velocity of the spin-wave excitations, we can see that these modes cross into the bottom of the quasiparticle continuum at a wave vector

$$q_o\sim\sqrt{\Delta_g/D}\,a^{-1}, \quad (5.33)$$

where a is the lattice parameter. This is much smaller than the size of the Brillouin zone so long-wavelength fluctuations of the order parameter will not lead to a dramatic reduction in its magnitude. The length scale

$$\xi\sim a\sqrt{D/\Delta_g} \quad (5.34)$$

thus plays the role of the coherence length for the odd-frequency paired state. On length scales shorter than ξ, and frequencies greater than

$$\omega\sim\Delta_g, \quad (5.35)$$

this system will behave much in the way of a single Kondo impurity. The development of coherence on longer length scales provides a vital cutoff to the infrared fluctuations that destroy the condensate in a single-impurity model.[47,48]

VI. EFFECT OF COHERENCE FACTORS ON LOCAL RESPONSE FUNCTIONS

The unusual nature of the coherence factors in the quasiparticle excitations have interesting consequences for the low-frequency response of the conduction electrons. Of particular interest here are the local dynamical spin and charge susceptibilities

$$\chi^c(\omega) = -i\int_0^\infty dt \langle [\rho_c(t), \rho_c(0)] \rangle e^{i\omega t} , \quad (6.1)$$

$$\chi^s_{ab}(\omega) = -i\int_0^\infty dt \langle [S_a(t), S_b(0)] \rangle e^{i\omega t} . \quad (6.2)$$

These functions are directly related to the ultrasonic attenuation, $\alpha_s(T)$, and the NMR relaxation rate, $1/T_1$,

$$\alpha_s(T) = \lambda_1 \lim_{\omega \to 0} \left[\frac{\chi^{c\prime\prime}(\omega)}{\omega} \right] ,$$

$$\frac{1}{T_1}(\hat{b}) = \lambda_2 \lim_{\omega \to 0} \left[\frac{\chi''_{+-}(\omega)}{\omega} \right] , \quad (6.3)$$

$$\chi_{+-}(\omega) = \mathrm{Tr}[(\underline{1} - \hat{b}\hat{b})\underline{\chi}^s(\omega)]$$

associated with the conduction electrons. Let us focus on contributions to these response functions derived from the gapless excitations in the "up-" spin band of our toy model.

The imaginary part of the local spin or charge response function of these excitations is given by

$$\frac{\chi^c(\omega)}{\omega} = \frac{4\chi^s_{zz}(\omega)}{\omega}$$
$$= \pi \sum_{\mathbf{k}_1, \mathbf{k}_2} |\langle \mathbf{k}_1 | \rho_{\mathbf{k}_2 - \mathbf{k}_1} | \mathbf{k}_2 \rangle|^2 \times \frac{[f(E_{\mathbf{k}_1}) - f(E_{\mathbf{k}_2})]}{\omega} \times \delta[(E_{\mathbf{k}_2} - E_{\mathbf{k}_1}) - \omega] . \quad (6.4)$$

(The only component of the susceptibility matrix which couples to the low-energy quasiparticles is χ^s_{zz}.) Since the coherence factors grow linearly in the energy

$$\left\langle \mathbf{k}- \left| \begin{Bmatrix} \rho_{\mathbf{q}} \\ \sigma^z_{\mathbf{q}} \end{Bmatrix} \right| \mathbf{k}^+ \right\rangle \sim \sqrt{Z_1 Z_2}(\omega_{\mathbf{k}^+} + \omega_{\mathbf{k}^-}) \left[\frac{\mu}{V^2} \right] . \quad (6.5)$$

The low-energy form of this response function is given by

$$\frac{\chi^c(\omega)}{\omega} = \frac{4\chi^s_{zz}(\omega)}{\omega}$$
$$= \pi \int dE\, N^*(E_+) Z(E_+) N^*(E_-) Z(E_-) \{ \cdots \} , \quad (6.6)$$
$$\{ \cdots \} = \left[\frac{f(E_-) - f(E_+)}{\omega} \right] \left[\frac{(E_+ + E_-)\mu}{V^2} \right]^2 ,$$

where $E_\pm = E \pm \omega/2$. The density of states of the quasiparticles is $N^*(E) = (\rho/2) Z^{-1}(E)$, thus at low temperatures and frequencies

$$\chi^c(\omega)/\omega = 4\chi^s_{zz}(\omega)/\omega = \frac{\pi\rho^2\mu^2}{4} \left[\frac{\omega^2 + (2\pi T)^2}{V^4} \right] . \quad (6.7)$$

This quadratic temperature and frequency dependence of the local charge and spin responses results from the unique energy dependence of the spin and charge matrix elements, and the neutrality and spinless character of excitations at the Fermi surface (Fig. 10). In a more conventional superconductor, where gapless excitations carry charge and spin, these matrix elements would be unity at the Fermi energy, and this kind of quadratic behavior can only be produced by a *linear* density of states. A quadratic growth of the dynamic spin and charge susceptibility results in characteristic T^3 response of the NMR relaxation rate (Fig. 1)

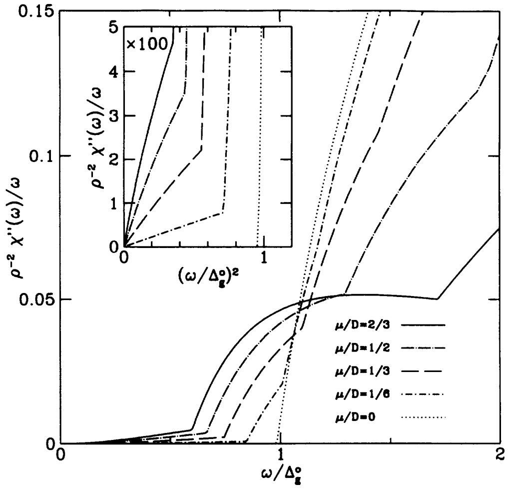


FIG. 10. Local dynamic spin susceptibility of the odd-frequency state for various values of μ/D. Inset details midgap response that grows quadratically with the frequency, due to linear spin coherence factors.

$$\frac{1}{T_1 T} \propto \left[\frac{\mu}{D} \right]^2 \left[\frac{T}{T_K} \right]^2 \quad (6.8)$$

and a T^2 response of the ultrasonic attenuation rate

$$\alpha_s(T) \propto \left[\frac{\mu}{D} \right]^2 \left[\frac{T}{T_K} \right]^2 . \quad (6.9)$$

This property of the odd-frequency paired state is of particular interest because power-law behavior of the above variety is observed in heavy-fermion systems. Conventionally, it is ascribed to *d*-wave pairing and gaps vanishing along lines of the Fermi surface. Our odd-paired state offers the interesting alternative description of this as a matrix element effect.

Let us now consider the detailed predictions of our model for the NMR relaxation rate. In general, there are two spin relaxation processes in heavy-fermion compounds: a relaxation rate associated with the conduction electrons

$$\left. \frac{1}{T_1 T} \right|_{\mathrm{cond}} = \lambda_2 \lim_{\nu \to 0} \left[\frac{\chi^{-+\prime\prime}_{\mathrm{cond}}(\nu)}{\nu} \right] ,$$
$$\chi^{-+}_{\mathrm{cond}}(\nu) = -i \int_0^\infty dt \exp(-i\omega t) \langle [S_c^-(t), S_c^+(0)] \rangle , \quad (6.10)$$

and a relaxation rate associated with the local moments, given by

$$\frac{1}{T_1 T}\Bigg|_f = \lambda_2 \lim_{\nu\to 0}\left[\frac{\chi_f^{-+''}(\nu)}{\nu}\right] ,$$
$$\chi_f^{-+}(\nu) = -i\int_0^\infty \exp(-i\omega t)\langle [S_f^-(t), S_f^+(0)]\rangle , \tag{6.11}$$

where S_c and S_f refer to a conduction or f spin at a given site. Existing NMR relaxation experiments have focused exclusively on relaxation at a nucleus in the surrounding conduction sea, on the assumption that the NMR relaxation rate at an actinide or rare-earth nucleus will be too large to resolve the broadened linewidth. In our model, these two relaxation rates differ qualitatively: the relaxation associated with the conduction states gives a T^3 response, whereas the relaxation associated with the heavy-fermion site vanishes exponentially at low temperatures, predicting that the nuclear line will narrow sufficiently to be resolved in the superconducting phase. Here we specifically calculate these two relaxation rates.

Let us first examine the gapless spin relaxation associated with the conduction electrons: this is determined by the z component of the dynamical spin susceptibility

$$\chi_{zz}^s(i\omega_n) = \langle S_z^c(i\omega_n) S_z^c(-i\omega_n)\rangle = \frac{1}{4}\sum_{\sigma=\pm}\langle \rho_{c\sigma}(i\omega_n)\rho_{c\sigma}(-i\omega_n)\rangle . \tag{6.12}$$

We may now write

$$\chi_{zz}^s(i\nu_n) = -\frac{T\rho^2}{16}\sum_{i\omega_n}\mathrm{Tr}[\mathcal{G}_\uparrow(i\nu_n + i\omega_n)\tau_3\mathcal{G}_\uparrow(i\omega_n)\tau_3] , \tag{6.13}$$

where we have used the summations over momentum to replace the "up" conduction propagators by the corresponding local propagator [Eq. (3.31)]

$$\frac{1}{\rho}\sum_{\mathbf{k}}\mathcal{G}_{\mathbf{k}\uparrow}(\omega+i\delta) = \frac{1}{2}\sum_\alpha \rho_{\uparrow\alpha}(\omega)\left\{-1 + \frac{\alpha(-\Delta_\omega\tau_1 - \mu\tau_3)}{E_\omega}\right\} , \tag{6.14}$$

where

$$E_\omega = \mathrm{sgn}(\omega)\sqrt{\Delta_\omega^2+\mu^2} ,$$
$$\rho_{\uparrow\alpha}(\omega) = (1/\rho)\mathrm{Im}[F_{\uparrow\alpha}(\omega+i\delta)] . \tag{6.15}$$

This spectral density can be used to carry out the Matsubara frequency convolution. We can consider the $\alpha=+$ term only, since it corresponds to the gapless excitations. The final expression for the imaginary part of the low-energy spin response is

$$\frac{\chi_{zz}^{s''}(\omega)}{\omega} = -\frac{\pi\rho^2}{32}\int dx\, \rho_{\uparrow +}(x)\rho_{\uparrow +}(x-\omega) \times \frac{f(x)-f(x-\omega)}{\omega}\{\cdots\} ,$$
$$\{\cdots\} = \left\{1 - \frac{\Delta_x\Delta_{x-\omega} - \mu^2}{E_x E_{x-\omega}}\right\} . \tag{6.16}$$

At low energies, the energy dependence of the magnetic relaxation is governed by the linear energy dependence of the spin coherence factors. The low-energy imaginary part of the susceptibility is hence quadratic in the external frequency,

$$\frac{\chi_{zz}^{s''}(\omega)}{\omega} = \frac{\pi\rho^2}{48}\left[\frac{\mu}{D}\right]^2\left[\frac{\omega}{T_K}\right]^2 . \tag{6.17}$$

This, in turn, leads to an NMR relaxation rate that is proportional to T^3:

$$\frac{1}{T_1 T} = \lambda_1\frac{\pi\rho^2}{48}\left[\frac{\mu}{D}\right]^2\left[\frac{2\pi T}{T_K}\right]^2 . \tag{6.18}$$

Let us now examine the spin relaxation rate of the f spins. Writing

$$S_f^+ = \sqrt{2}\eta^3 f^\dagger ,$$
$$S_f^- = \sqrt{2} f^\dagger\eta^3 , \quad f^\dagger = \frac{1}{\sqrt{2}}(\eta^1 + i\eta^2) , \tag{6.19}$$

we can define

$$G^\perp(\omega) = \langle f(\omega) f^\dagger(\omega)\rangle = \int \frac{d\omega'}{\omega-\omega'}\rho^\perp(\omega) ,$$
$$G^3(\omega) = \langle \eta^3(\omega)\eta^3(-\omega)\rangle = \int\frac{d\omega'}{\omega-\omega'}\rho^3(\omega) . \tag{6.20}$$

Then at the mean-field level, the local dynamical susceptibility of the f spins is

$$\chi_f^{-+}(\nu) = -2T\sum_{\nu=i\omega_n} G^\perp(\omega)G^3(\omega+\nu) . \tag{6.21}$$

Carrying out the sum over Matsubara frequencies, we then find that

$$\lim_{\nu\to 0}\left[\frac{\chi_f^{-+''}(\nu)}{\nu}\right] = 2\pi\int d\omega\,\rho^\perp(\omega)\rho^3(\omega)\left[-\frac{\partial f(\omega)}{\partial\omega}\right] . \tag{6.22}$$

The essential features of this relaxation rate are captured by the situation at half filling, where

$$2\rho^3(\omega) = \rho^\perp(\omega) = \left[\frac{V^2}{\omega^2}\right]\rho . \tag{6.23}$$

To leading exponential accuracy, the relaxation rate is then

$$\frac{1}{T_1 T}\Bigg|_f = \frac{\alpha}{\Delta_g^2}e^{-\Delta_g/T} \quad (\alpha = 2\pi\lambda_f[\rho D]^2) . \tag{6.24}$$

This exponential relaxation at the heavy-fermion site is a reflection of the "s-wave" character of the odd-frequency triplet pairing: condensation between the f spins and the conduction electrons builds a sharp gap in the excitation spectrum of the f spins. We refer the reader to Fig. 1, which contrasts the NMR relaxation rates at the heavy-fermion and conduction electron sites for various values of the chemical potential.

The key difference between the d-wave and odd-frequency description is that the former relies on a node in momentum space, whereas the latter relies on a node in frequency space. For this reason, we expect that odd-frequency pairing is rather insensitive to elastic scattering. This point can be illustrated in the following general way. Let us consider a general odd-frequency paired state, where the pairing self-energy takes the form

$$\underline{\Sigma}(\omega;x,x')=\zeta(x)\frac{V_o^2}{\omega}\mathcal{P}(x)\delta_{xx'}\ ,$$
$$\underline{\mathcal{P}}=\tfrac{1}{4}[3(\underline{1})-d_{ab}(x)\sigma^a\otimes\tau^b]\ . \tag{6.25}$$

In this expression, the amplitude $V_o^2\zeta(x)$ of the resonant scattering and the orientation $d_{ab}=\frac{1}{2}Z^\dagger(x)\sigma_a\tau_b Z(x)$ of the triplet order parameter may be site dependent. The component of the conduction electron states which does not directly couple to the resonant pairing, $\Psi_o(x)$, may be projected out of the conduction electron spinor as follows:

$$\Psi_o(x)=\underline{p}(x)\Psi(x)\ ,$$
$$\underline{p}(x)=\underline{1}-\underline{\mathcal{P}}(x)=\tfrac{1}{4}[(\underline{1})+d_{ab}(x)\sigma^a\otimes\tau^b]\ . \tag{6.26}$$

This component experiences an indirect effect of the resonant pairing through mixing with the directly scattered components.

Consider a general conduction electron band with disorder, described by the Hamiltonian

$$H_c=\frac{1}{2}\sum\Psi^\dagger(x)\mathcal{H}(x,x')\Psi(x')\ . \tag{6.27}$$

Let us project out the parts of the conduction electron Hamiltonian that couple directly, or indirectly to the resonant scattering, writing

$$\left[\begin{array}{c|c} h_{xx'} & \alpha_{x,x'} \\ \hline \alpha^\dagger_{x,x'} & H_{xx'}\end{array}\right] = \left[\begin{array}{c|c} \underline{p}(x) & \\ \hline & \mathcal{P}(x)\end{array}\right]\mathcal{H}(x,x')\left[\begin{array}{c|c} \underline{p}(x) & \\ \hline & \mathcal{P}(x)\end{array}\right]\ . \tag{6.28}$$

The conduction electron Green's function can then be written

$$\underline{\mathcal{G}}(\omega)=\left[\omega-\underline{\mathcal{H}}-\frac{V_o^2}{\omega}\underline{\zeta}\underline{\mathcal{P}}\right]^{-1}\quad[\underline{\zeta}_{x,x'}=\zeta(x)\delta_{x,x'}]\ , \tag{6.29}$$

where all subscripts have been omitted. The projected component of the conduction electron propagator for those states that do not directly couple to the resonant scattering is then given by

$$\underline{G}_o^{-1}(\omega)=\omega-\underline{h}-\underline{\alpha}\left[\omega-H-\frac{V_o^2}{\omega}\underline{\zeta}\right]^{-1}\underline{\alpha}^\dagger\ . \tag{6.30}$$

Though these states do not directly couple to the resonant scattering, they couple indirectly because of the off-diagonal terms in the Hamiltonian that mix them with the resonantly scattered states. At low energies, the resonant scattering dominates the "self-energy" correction in the propagator, which then becomes

$$\underline{G}_o^{-1}(\omega)=\underline{Z}^{-1}\omega-\underline{h}\ ,$$
$$\underline{Z}^{-1}=\left[1+\frac{\underline{\alpha}\underline{\zeta}^{-1}\underline{\alpha}^\dagger}{V_o^2}\right]\ . \tag{6.31}$$

Notice that the effect of the resonant scattering is to introduce a wave-function renormalization into the propagator. Low-energy eigenstates are set by the determinantal equation

$$\mathrm{Det}[\underline{G}_o^{-1}]=0\ . \tag{6.32}$$

Clearly then, if there are zero-energy eigenstates of the projected Hamiltonian

$$\underline{h}(x,x')\xi_\lambda(x')=0\ , \tag{6.33}$$

then these will give rise to zeros in this determinant. In other words, the projective character of the resonant scattering means that the indirectly coupled zero-energy states form zero-energy excitations of the *complete* Hamiltonian. Suppose we define the Majorana conduction electron states as

$$a_\lambda^\dagger=\sum_x\psi_o(x)\xi_\lambda(x)\ . \tag{6.34}$$

Then their propagator will be given by

$$\langle a(\omega)a^\dagger(\omega)\rangle=\xi_\lambda^\dagger\underline{G}_o(\omega)\xi_\lambda=\frac{Z_\lambda}{\omega}\ , \tag{6.35}$$

where the pole strength Z_λ is

$$Z_\lambda=\left[1+\xi_\lambda^\dagger\frac{\underline{\alpha}\underline{\zeta}^{-1}\underline{\alpha}^\dagger}{V_o^2}\xi_\lambda\right]^{-1}\ . \tag{6.36}$$

Thus, the zero-energy eigenstates of the complete Hamiltonian will have the form

$$\tilde{a}_\lambda^\dagger=\sqrt{Z_\lambda}\sum_x\psi_o(x)\xi_\lambda(x)+\cdots\ , \tag{6.37}$$

where the residual part of strength $\sqrt{(1-Z_\lambda)}$ is carried entirely by the Majorana spin fermions. In general then, the off-diagonal coupling between the indirectly and directly scattered states leads to a reduction in the conduction character of the Majorana zero modes, and a corresponding enhancement of the density of gapless excitations:

$$N^*(0)=\left[\frac{\rho}{2}\right]\langle Z_\lambda^{-1}\rangle_\lambda\ . \tag{6.38}$$

The important point, however, is that despite these effects, the gapless excitations remain Majorana fermions: the spin and charge operators are completely off-diagonal at the Fermi surface, and coherence factors must consistently vanish in this region.

To provide a specific example, consider the generalization of our toy model with a random chemical potential

$$H_c=\frac{1}{2}\sum_{\mathbf{k}}\Psi_{\mathbf{k}}^\dagger\epsilon_{\mathbf{k}}\Psi_{\mathbf{k}}-\frac{1}{2}\sum_x\Psi^\dagger(x)\mu(x)\underline{\tau}_3\Psi(x)\ . \tag{6.39}$$

The chemical potential term can be identified as the off-diagonal coupling, whereas the kinetic-energy term commutes with the projection. The Z factor for a gapless plane wave $\xi_{\mathbf{k}}(x)=(1/\sqrt{N})e^{i\mathbf{k}\cdot\mathbf{x}}Z_{\mathbf{k}}$ is then

$$Z_{\mathbf{k}}^{-1}=[1+\langle\mu^2(x)\rangle/V_o^2] , \qquad (6.40)$$

which gives rise to an enhancement of the gapless density of states given by

$$N^*(0)=\frac{\rho}{2}[1+\langle\mu^2(x)\rangle/V_o^2] , \qquad (6.41)$$

where for weak scattering we have ignored the fluctuations in the strength of the resonant scattering potential that will be induced by the disorder. Thus, we see that disorder *enhances* the density of states but sustains the electric and magnetic neutrality of the Fermi surface.

VII. INTERPLAY WITH MAGNETISM

In this section we discuss some of the magnetic aspects of the odd-frequency state. Even in our toy model, where we have not included any detailed effects of band structure or anisotropy, there are a variety of locally stable phases where the order parameter is commensurately staggered. Quite generally, as we now show, the odd-frequency state will develop an ordered magnetic moment, aligned parallel to the $\hat{d}^3$ vector, giving rise to the coexistence of antiferromagnetism and superconductivity.

We begin our discussion by returning to the simplest example, where the $\hat{d}^3$ vector is uniformly oriented, giving rise to a state with ferromagnetic correlations. We will generalize our discussions to a more realistic antiferromagnetically ordered case at the end of the section. When the conduction band is half filled, and hence completely particle-hole symmetric, the odd-frequency paired state is magnetically isotropic and both static magnetic order and static pair correlations are absent $\langle\mathbf{S}\rangle=0$, $\langle\tau_j\rangle=0$ at half filling. In this state, there is long-range order with an order parameter

$$\langle S^a(x)\tau^b(x)\rangle=2\frac{V^2}{J^2}[\hat{d}_b(x)]^a , \qquad (7.1)$$

where $\mathbf{S}(x)=\mathbf{S}_c(x)+\mathbf{S}_f(x)$ is the total moment at site x, and $\tau(x)$ is the conduction electron isospin at site x. Odd-frequency triplet pairing is thus seen to strongly couple spin and pair correlations. Clearly, however, these cross correlations induce anomalous response functions, coupling the development of charge correlations to the application of a magnetic field or the development of magnetic correlations to the application of a chemical potential or pairing field. To study this effect, we introduce the spin-charge susceptibility

$$\chi^{ab}(\kappa)=\langle S^a(\kappa)\tau^b(-\kappa)\rangle , \qquad (7.2)$$

where the static susceptibility $\underline{\chi}(0)$ is of particular interest. In the vicinity of half filling, the state is completely isotropic in spin and isospin space, and we then expect

$$\chi^{ab}=\chi_o d^{ab} . \qquad (7.3)$$

Thus, once the system is doped ($\mu\neq 0$), the presence of a cross correlation between the charge and spin degrees of freedom leads to the development of a magnetic moment and strong anisotropy

$$\mathbf{M}\sim\chi_o\hat{d}^3\mu . \qquad (7.4)$$

We may calculate χ_o very simply as follows. Let us choose $\hat{d}^3=\hat{z}$. The coupling of the magnetic field is given by

$$H_B=-\sum_j \mathbf{B}\cdot\left\{\psi^\dagger(j)\left[\frac{\sigma}{2}\right]\psi(j)-\frac{i}{2}\boldsymbol{\eta}_j\times\boldsymbol{\eta}_j\right\} . \qquad (7.5)$$

Thus, the total magnetic moment in the $\hat{z}$ direction per site is

$$M=\langle\tfrac{1}{2}(n_{c\uparrow}-n_{c\downarrow})-i\eta_1(j)\eta_2(j)\rangle$$
$$=\langle\tfrac{1}{2}(n_{c\uparrow}-n_{c\downarrow})+(1/2-n_{\eta\downarrow})\rangle , \qquad (7.6)$$

where $n_{c\sigma}$, ($\sigma=\uparrow,\downarrow$) is the number of "up" or "down" conduction electrons per site and following the notation of Eq. (3.18), $n_{\eta\downarrow}=(1/N_{\text{sites}})\sum_{\mathbf{k}}\eta^\dagger_{\mathbf{k}\downarrow}\eta_{\mathbf{k}\downarrow}$ is the number of "down" Majorana fermions per site. Now note that the down Majorana electrons are hybridized with the down conduction electrons to produce a completely filled hybridized band, with one electron per unit cell. Thus, in the ground state, $\langle n_\eta+n_{c\downarrow}\rangle=1$ per site, so

$$M_z=\tfrac{1}{2}\langle n_{c\uparrow}+n_{c\downarrow}\rangle-\tfrac{1}{2} \qquad (7.7)$$

per site. Since the local moments leave the conduction electron density essentially unchanged, $\langle n_{c\uparrow}+n_{c\downarrow}-1\rangle=2\rho\mu$, giving

$$M_z=\rho\mu \qquad (7.8)$$

and

$$\chi_o=\rho+O(T_K/D) . \qquad (7.9)$$

A departure from particle-hole symmetry $\delta\mu$ thus generates an ordered (ferromagnetic) moment of strength

$$\mathbf{M}(x)=\delta\mu\rho\hat{d}^3(x) . \qquad (7.10)$$

In a similar fashion, an application of a magnetic field will influence the charge and pair correlations: a field along the $\hat{d}_3$ direction will develop a charge density,

$$\rho(x)=\rho B_z(x) . \qquad (7.11)$$

More remarkably, a *transverse* magnetic field $\mathbf{B}=B_\perp\hat{d}^l$ ($l=1,2$) will induce a conventional pairing field of magnitude

$$\langle\psi^\dagger_\uparrow\psi{\downarrow}^\dagger\rangle\sim\rho_o B_\perp . \qquad (7.12)$$

This leads to a possible field-dependent Josephson coupling with conventional superconductors.

Even in this ferromagnetically ordered state, there are strong antiferromagnetic correlations. To illustrate this point, consider the case where $\mu=0$. Here, the main contribution to the magnetic susceptibility is provided by the local moments, and may be calculated from the spatial correlations of the Majorana fields. Low-frequency properties of the local moments are determined by excitations across the indirect gap at wave vectors $\mathbf{q}=\pm\mathbf{Q}/2$. In the vicinity of the gap, the Majorana fermions can be expanded as shown in Eqs. (3.5) and (3.6). In momentum space, the Majorana propagators have the form

$$\langle \eta^a(\kappa)\eta^b(-\kappa)\rangle=\delta_{ab}D(\kappa)\ ,\qquad D(\kappa)=\frac{i\omega_n-\epsilon_{\mathbf{k}}}{[i\omega_n(i\omega_n-\epsilon_{\mathbf{k}})-V^2]}\ , \tag{7.13}$$

so that

$$\mathrm{Im}D(\mathbf{k},\omega-i\delta)=\frac{V^2}{V^2+\omega^2}\pi\delta(\omega-\omega_{\mathbf{q}})\ . \tag{7.14}$$

The spin correlations are determined from the product of two Majorana propagators:

$$\langle S^a(q)S^b(-q)\rangle=\delta^{ab}\chi(q)=\delta^{ab}\frac{T}{2}\sum_{\kappa}D(q/2+\kappa)D(\kappa-q/2)\ . \tag{7.15}$$

At low frequencies, this is governed by excitations in the vicinity of the indirect gap, where the quasiparticle spectrum is parabolic $\omega_q=\pm\Delta_g+(q\pm\mathbf{Q}/2)^2/2m^*$, $m^*=(D/T_K)m$, and m is the electron mass at the band edge. Using this parabolic approximation to carry out the momentum space integrals gives

$$\mathrm{Im}\chi(\mathbf{q},\omega+i\delta)\approx\delta^{ab}\frac{(m^*)^{3/2}}{(2\pi)^2}\left[\frac{V^2}{V^2+(\omega/2)^2}\right]\times\sqrt{\omega-\Delta_{\mathbf{q}}}\,\Theta(\omega-\Delta_{\mathbf{q}})\ ,\qquad \Delta_{\mathbf{q}}=2\Delta_g+\frac{(\mathbf{q}+\mathbf{Q})^2}{4m^*}\ . \tag{7.16}$$

In other words, independently of the ordered magnetic moments, there is a large amount of spin-fluctuation spectral weight above the superconducting gap at the antiferromagnetic zone vector. This general feature survives when we come to consider other configurations of $\hat{d}^3(x)$.

Let us now consider the possibility of more general, staggered configurations of $\hat{d}^3$. Take the more general ansatz for the mean-field order parameter

$$z(\mathbf{x})=e^{-i(1/2)\mathbf{x}\cdot(\mathbf{Q}+\mathbf{P}\underline{\sigma}_1)}z_o,\ z_o\equiv\begin{bmatrix}1\\0\end{bmatrix}\ ,\qquad \underline{\mathcal{M}}(x)=\begin{bmatrix}\hat{d}_1(x)\\ \hat{d}_2(x)\\ \hat{d}_3(x)\end{bmatrix}=\begin{bmatrix}\hat{d}_1\cos[\mathbf{Q}\cdot\mathbf{x}]\\ \hat{d}_2\cos[(\mathbf{Q}+\mathbf{P})\cdot\mathbf{x}]\\ \hat{d}_3\cos[(\mathbf{P}\cdot\mathbf{x})]\end{bmatrix}\ , \tag{7.17}$$

where $\mathbf{P}$ and $\mathbf{Q}$ are commensurate vectors.

As before, we can redefine the conduction electron states to take account of the staggered order,

$$z_j=e^{(i/2)\mathbf{x}_j\cdot(\mathbf{Q}+\mathbf{P}\underline{\sigma}_1)}\tilde{z}_j\ \ (\mathcal{Z}_j=e^{(i/2)\mathbf{x}_j\cdot(\mathbf{Q}\underline{\tau}_3+\mathbf{P}\underline{\sigma}_1)}\tilde{\mathcal{Z}}_j)\ ,\qquad \Psi_j=e^{(i/2)\mathbf{x}_j\cdot(\mathbf{Q}\underline{\tau}_3+\mathbf{P}\sigma_1)}\tilde{\Psi}_j\ . \tag{7.18}$$

The conduction electron Hamiltonian can then be written

$$H_c=\sum_{\mathbf{k}\in\frac{1}{2}\mathrm{BZ}}\Psi_{\mathbf{k}}^{\dagger}[(\epsilon[\mathbf{k}-\mathbf{Q}/2\underline{\tau}_3-\mathbf{P}/2\underline{\sigma}_1]-\mu)\underline{\tau}_3]\Psi_{\mathbf{k}}\ , \tag{7.19}$$

where the kinetic-energy term can be expanded as

$$[\epsilon(\mathbf{k}-\mathbf{Q}/2\underline{\tau}_3-\mathbf{P}/2\underline{\sigma}_1)-\mu]\underline{\tau}_3=\frac{1}{4}\sum_{\alpha,\beta=\pm1}\{(\underline{\tau}_3+\alpha)(1+\beta\underline{\sigma}_1)\epsilon[\mathbf{k}-\alpha\mathbf{Q}/2-\beta\mathbf{Q}/2]\}-\mu\underline{\tau}_3=[\tilde{\epsilon}_{\mathbf{k}}^{o}+\tilde{\epsilon}_{\mathbf{k}}^{1}\underline{\sigma}_1]-[\mu_{\mathbf{k}}^{0}+\mu_{\mathbf{k}}^{1}\underline{\sigma}_1]\underline{\tau}_3\ . \tag{7.20}$$

From the discussion of Sec. III, we know that gapless excitations will develop on the "Fermi surfaces" described by

$$\tilde{\epsilon}_{\mathbf{k}}^{0}=\frac{1}{4}\sum_{\alpha,\beta=\pm1}\alpha\epsilon[\mathbf{k}-\alpha\mathbf{Q}/2-\beta\mathbf{P}/2]=0\ . \tag{7.21}$$

To make our example more specific, consider the case where

$$\epsilon_{\mathbf{k}}=-2t[c_x+c_y+c_z]\ \ (c_l=\cos[k_l],\ l=1,2,3)\ ,\qquad \mathbf{Q}=(\pi,\pi,\pi),\ \ \mathbf{P}=(\pi,0,0)\ , \tag{7.22}$$

corresponding to a staggered $\hat{d}^3$ vector in the x direction. In this case,

$$\tilde{\epsilon}_{\mathbf{k}}^{o}=-2t[s_y+s_z]\ \ (s_l=\sin[k_l],\ \ l=1,2,3)\ ,\qquad \tilde{\epsilon}_{\mathbf{k}}^{1}=2tc_x\ ,\qquad \mu_{\mathbf{k}}^{o}=\mu,\ \ \mu_{\mathbf{k}}^{1}=0\ . \tag{7.23}$$

The gapless modes lie on a tube with a square cross section $[s_y+s_z]=0$ and the spectrum is given by

$$\mathrm{Det}[\underline{G}_{\uparrow}^{-1}(\omega)\underline{G}_{\downarrow}^{-1}(\omega)-[\epsilon_{\mathbf{k}}^{1}]^2\underline{1}]=0\ ,\qquad \underline{G}_{\uparrow}^{-1}(\omega)=[\omega-\epsilon_{\mathbf{k}}^{o}-\Delta_{\omega}(1-\tau_1)+\mu\tau_3]\ ,\qquad \underline{G}_{\downarrow}^{-1}(\omega)=[\omega-\epsilon_{\mathbf{k}}^{o}-2\Delta_{\omega}+\mu\tau_3]\ . \tag{7.24}$$

After a short calculation the corresponding mass renormalization of the gapless quasiparticles is found to be

$$\frac{m}{m^*}=\left[1+\left[\frac{\mu^2+(2tc_x)^2}{V^2}\right]\right]\ . \tag{7.25}$$

In Fig. 11, we show the mean-field ground-state energy as a function of $\mathbf{P}=(P_x,P_y,P_z)$, clearly showing the development of local minima at the commensurate points in the Brillouin zone. At each of these points the odd-frequency state will develop a staggered magnetization with wave vector $\mathbf{P}$ and approximate magnitude $M\sim\rho\mu$.

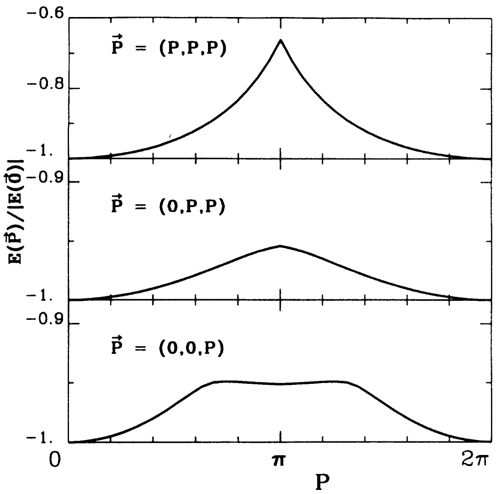


FIG. 11. Dependence of mean-field free energy on the magnetic wave vector **P** in three dimensions. In three dimensions, the state at $\mathbf{P}=(\pi,0,0)$ is locally stable.

In practice, we would argue that the small differences in energy between these different commensurate states will depend on several factors that are not included in the toy model. It is interesting to note that in two dimensions, the toy model predicts that a $\mathbf{P}=(\pi,0)$ state is more stable than the $\mathbf{P}=(\pi,\pi)$ state. The important point, however, is that the mean-field energy of these magnetic phases is close in energy to the uniform state and furthermore, is locally stable. We may conclude that this type of odd-frequency pairing can homogeneously coexist with antiferromagnetism. The local moments participate in both the spin and the pair condensate.

VIII. CRITIQUE AND DISCUSSION

Our paper has presented a "toy" realization of odd-frequency pairing, with the aim of elucidating its key properties. In this section, we discuss the odd-frequency state in a more general setting and examine the possibility that this kind of paired state might be applicable to heavy fermions.

One of the most dramatic features of the theory is the projective character of the resonant pairing self-energy:

$$\underline{\Sigma}(\omega)=\frac{V^2}{\omega}\underline{\mathcal{P}}\ ,\qquad \underline{\mathcal{P}}=\tfrac{1}{4}[(\underline{3})-d_{ab}\sigma^a\otimes\tau^b]\ . \tag{8.1}$$

Can we understand this feature in a more general context, outside the restrictive realm of the Kondo model, and our Majorana treatment? Let us consider the possible extension of our odd-paired state within an Anderson model for heavy fermions, with an on-site repulsion term

$$H_I=\tfrac{1}{2}U(n-1)^2 \tag{8.2}$$

at each magnetic site. Highly correlated states minimize this on-site interaction energy, tending to produce local moment states where $n=1$. It is quite useful to examine this constraint in terms of the correlations between the charge (isospin) and spin of the localized states. If we expand the localized f electron in terms of its four real components

$$\begin{bmatrix} f_\uparrow \\ f_\downarrow \end{bmatrix}=\frac{1}{\sqrt{2}}[f^0+i\mathbf{f}\cdot\boldsymbol{\sigma}]z\ , \tag{8.3}$$

where

$$z=\begin{bmatrix} z_\uparrow \\ z_\downarrow \end{bmatrix}$$

is a unit spinor, then the interaction may be written as a symmetric product of all four fields[49]

$$\begin{aligned} H_I&=U[(\tau_3)^2-(S_z)^2]+\frac{U}{4}\\ &=U[(if^0f^1)(if^2f^3)+\tfrac{1}{4}]\ . \end{aligned} \tag{8.4}$$

On a lattice, the interaction between the electrons can then be written

$$S_I=-U\sum_\kappa\{f^0_{\kappa_0}f^1_{\kappa_1}f^2_{\kappa_2}f^3_{\kappa_3}\}\delta_{\kappa_0+\kappa_1+\kappa_2+\kappa_3}\ , \tag{8.5}$$

where we use the Fourier-transformed operators

$$f^a(\kappa)=\frac{1}{\sqrt{\beta N}}\sum_j\int d\tau e^{-i\kappa\cdot X}f^a(X)\ ,\qquad \kappa\cdot X\equiv\mathbf{k}\cdot\mathbf{R}_j-\omega_n\tau \tag{8.6}$$

and it is understood that all time coordinates are ultimately to be time ordered.

A way to reduce the on-site correlation energy is to develop a correlated state where certain Majorana components of the f state are *absent.* Remarkably, the operator that projects out the zeroth component at wave vector κ

$$f^0(\kappa)=\frac{1}{\sqrt{2}}[z^\dagger f(\kappa)+f^\dagger(-\kappa)z] \tag{8.7}$$

is a *one-particle* operator

$$p_\kappa=f_o[\kappa]f_o[-\kappa]=\tfrac{1}{4}\mathcal{F}^\dagger_\kappa[\underline{1}+d_{ab}\sigma_a\otimes\tau_b]\mathcal{F}_\kappa\ , \tag{8.8}$$

where $d_{ab}=\frac{1}{2}\mathcal{Z}^\dagger\sigma_a\otimes\tau_b\mathcal{Z}$,

$$\mathcal{Z}=\begin{bmatrix} z \\ -i\sigma_2z^* \end{bmatrix}\ , \tag{8.9}$$

and

$$\mathcal{F}_\kappa=\begin{bmatrix} f_\kappa \\ -i\sigma_2f^*_{-\kappa} \end{bmatrix},\quad f_\kappa=\begin{bmatrix} f_{\kappa\uparrow} \\ f_{\kappa\downarrow} \end{bmatrix} \tag{8.10}$$

are the Balian-Werthamer four spinors for the f state and z spinor. The residual "vector" (1,2,3) components of the f states are projected out by the one-particle operator

$$\hat{\mathcal{P}}_\kappa=\sum_{j=1,3}f_j[-\kappa]f_j[\kappa]=1-p_\kappa=\mathcal{F}^\dagger_\kappa\underline{\mathcal{P}}\mathcal{F}_\kappa\ . \tag{8.11}$$

The Majorana character of this operator implies that it is antisymmetric

$$\hat{\mathcal{P}}_\kappa = -\hat{\mathcal{P}}_{-\kappa} . \quad (8.12)$$

The self-energy term that will selectively decouple Majorana components of the f electrons will have the general form

$$\underline{\Sigma}(\kappa) = \Delta(\kappa)\underline{\mathcal{P}} ,$$
$$S_I = \sum_\kappa \mathcal{F}^\dagger(\kappa)\underline{\Sigma}(\kappa)\mathcal{F}(\kappa) = \sum_\kappa \Delta(\kappa)\underline{\hat{\mathcal{P}}}_\kappa . \quad (8.13)$$

Since $\hat{\mathcal{P}}_\kappa$ is an odd function of κ, it follows that

$$\Delta(\kappa) = -\Delta(-\kappa) . \quad (8.14)$$

If the physics is local in time, then the frequency dependence of $\Delta(\kappa)$ can be dropped, leading to p-wave triplet pairing. However, if the momentum dependence of $\Delta(\kappa)$ is even, the frequency dependence is automatically *odd*, leading to odd-frequency pairing. In the simplest s-wave version of this pairing, the physics is spatially local, so that $\Delta(\kappa) = \Delta(\omega)$. This establishes an intimate connection between the projection of Majorana degrees of freedom from the ground state and the development of nodes in the wave function: when the physics is local, this projection results in a *node in time,* and the development of odd-frequency pairing.

A general spectral decomposition of $\Delta(\omega)$ will always contain a zero-frequency pole

$$\Delta(\omega) = \frac{Z}{\omega} + \omega \int \frac{d\nu}{\pi} \frac{A(\nu)}{\omega^2 - \nu^2} ,$$
$$\frac{1}{\pi}\text{Im}[\Delta(\omega - i\delta)] = Z\delta(\omega) + A(\omega) . \quad (8.15)$$

This pole is a unique feature of odd-frequency pairing: it suppresses the "vector" components of the f electron from the low-energy excitations, gaining correlation energy and decoupling a band of gapless singlet excitations. Our simple mean-field theory can be viewed as a dominant pole approximation to the pairing field. A pressing need for the near future is to show that such general constructions can lead to stable Eliashberg-type treatments of more general models, such as the finite-U Anderson lattice.

In its current form, our prototype for odd-frequency pairing is too simplistic to account for details of heavy-fermion behavior. We should like to list some important issues which need to be addressed in future developments.

(1) Magnetism. The toy model has shown that odd-frequency pairing has a propensity to coexist with magnetism. A more realistic model will need to take explicit account of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions and their role in establishing the detailed superconducting order.

(2) Normal phase. The normal phase of heavy-fermion superconductors, with its profusion of Fermi-liquid features, does not appear in the toy model. The Majorana formalism may be a poor starting point to recover the normal phase properties, and this suggests that we should seek a way to obtain the odd-frequency paired state within perturbation theory for the finite-U Anderson model, or perhaps the large-N approach to the heavy-fermion problem.

(3) Anisotropy. Measurements of the gap and ultrasound absorption[50,51] in UPt_3 show the presence of anisotropy in the order parameter and have been traditionally interpreted within a d-wave pairing scenario. These results *do not* reveal the temporal parity of the paired state, but tend to reinforce the conclusion that momentum anisotropy can not be ignored in a more advanced version of the model. Indeed, there is no reason not to contemplate the possibility of odd-frequency d-wave pairing.

(4) Power laws. Power laws in the temperature dependence of the specific heat and NMR relaxation rate of heavy-fermion compounds develop much closer to T_c than any simple mean-field theory can account for. One possibility is that dynamic pair-breaking effects have suppressed T_c significantly below the gap. Odd-frequency pairing accounts for the finite linear specific heats in heavy-fermion superconductors in terms of a band of excitations with vanishing coherence factors. At present, the toy model is *unable* to account for the T^2 term in C_V that is also seen. Fluctuation effects need to be examined carefully.

We should like to spend a moment discussing the long-wavelength properties of odd-frequency triplet paired states. The intimate relation between spin and pair degrees of freedom in this kind of state leads to rather interesting consequences in the Landau-Ginzburg theory. Suppose one considers the simple long-wavelength action discussed in Sec. V A:

$$F = \frac{1}{2}\int d^3x \left[\rho_\perp(\nabla \hat{n})^2 + \rho_s \left[\omega_3 - \frac{2e}{\hbar}\mathbf{A} \right]^2 + \frac{B^2}{\mu_o} \right]$$
$$- \frac{\rho_s}{l_o^2}\int d^3x (\hat{d}_3 \cdot \hat{z})^2 . \quad (8.16)$$

Then the anisotropy plays a vital role in establishing the topological stability of persistent currents. Unlike a conventional superconductor, the supercurrent is linked to the spin order and involves all three Euler angles of the order parameter. To see this, it is instructive to consider a loop of superconductor of length L, threaded by a solenoid. The supercurrent around the loop is given by

$$\mathbf{j}_s = \frac{2e}{\hbar}\rho_s \left[\omega_3 - \frac{2e}{\hbar}\mathbf{A} \right] ,$$
$$\omega_3 = \nabla\phi + \cos\theta \nabla\psi , \quad (8.17)$$

where (ϕ, θ, ψ) are the Euler angles defining the orientation of the triad d_{ab}. Notice that, unlike a conventional superconductor, the supercurrent involves *both* the U(1) phase ϕ and the orientation of the magnetic vector $\hat{d}$, defined by (θ, ψ). For a conventional superconductor the total phase change around the loop is a topological invariant

$$\Delta\phi = \int d\mathbf{r} \cdot \nabla\phi = 2\pi n \quad (8.18)$$

that is unchanged upon application of a flux through the solenoid, leading to a linear relation $j_s = -(4\pi e/hL)\rho_s(\Phi/\Phi_o)$ between the enclosed flux Φ and the supercurrent density j_s. In this superconductor, the analogous integral around the current loop is

$$\Delta\phi=\int d\mathbf{r}\cdot[\nabla\phi+\cos\theta\nabla\psi]=2\pi n+\Omega \ . \tag{8.19}$$

The second term

$$\Omega=\int d\mathbf{r}\cdot[\cos\theta\nabla\psi]=\int_S d\mathbf{S}\cdot(\epsilon_{ab}\nabla_a\hat{n}\times\nabla_b\hat{n}) \tag{8.20}$$

is the solid angle subtended by the $\hat{n}$ vector around the loop: this is *not* an invariant, and can change by multiples of 4π to relax the current. Unlike the U(1) superconductor, the only stable vortex configuration involves a net phase change of 2π around the loop: this is the so-called "Z_2" vortex of an SO(3) order parameter, and it has the property that two such vortices can be adiabatically deformed back to the vacuum (Fig. 12). Each Z_2 vortex pair reduces the effective flux through the solenoid by two flux quanta, thus the nonlinear current will be given by

$$j=\frac{2e}{hL}\rho_s\left[2\pi\frac{\Phi}{\Phi_o}-4\pi n_Z\right] , \tag{8.21}$$

where the number of Z_2 vortex pairs is

$$n_Z=\mathrm{Int}\left[\frac{\Phi}{2\Phi_o}+\frac{1}{2}\right] , \tag{8.22}$$

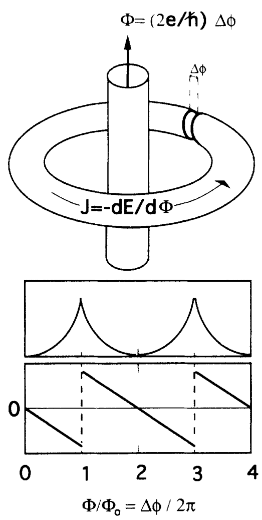


FIG. 12. Illustrating the energy dependence on the flux through a ring of odd-frequency triplet superconductor (no spin anisotropy). The phase ϕ displayed here refers to the phase of the charge $2e$ composite order parameter $g\mathcal{M}_\alpha^\beta(x)=\langle\tau_\alpha(x)S^\beta(x)\rangle$. When the flux through the loop exceeds one flux quantum, the system can relax the energy and supercurrent by rotating the axes of the order parameter into the third dimension, creating two Z_2 antivortices. This reduces the effective flux through the ring by two flux quanta, changing the sign of the supercurrent $J=-\partial E/\partial\phi$ and producing a sawtooth dependence of current on flux. The ground-state energy is a periodic, rather than a quadratic function of the applied flux. A macroscopic Meissner current cannot develop in response to the flux threading the loop unless spin anisotropy is added to prevent the rotation of the order parameter into the third dimension.

where Int(x) denotes the largest integer smaller than x. In this way, the current density around the loop can never exceed

$$j_o=\frac{(2\pi)}{L\Phi_o}\rho_s \tag{8.23}$$

and will never become macroscopic. Thus, without anisotropy, the critical current for the odd-frequency state is *zero*. Furthermore, if the flux through the solenoid is $\Phi=\int V(t)dt$, then the response to an oscillatory electric field will not occur at the driving frequency. This will eliminate the low-frequency linear Meissner response to macroscopic fields, removing the pole in the optical conductivity and producing an *apparent violation* of the linear response optical sum rule. This type of behavior is most likely to occur in the vicinity of particle-hole symmetry, and suggests that this half-filled state will more closely resemble an insulator, rather than a superconductor. This may be an interesting way of thinking about Kondo insulators,[52] where an anomalous reduction in the low-frequency oscillator strength of the optical conductivity has recently been reported.[53] As anisotropy is increased, a macroscopic free-energy barrier will have to be crossed in order to add pairs of Z_2 vortices to the superconducting state, restoring the linear Meissner response. This will lead to a nontrivial dependence of the critical current on anisotropy.

Pending further theoretical work, it appears that there may be some useful experiments on heavy-fermion superconductors that could help to compare the d-wave and odd-frequency scenarios. Two key predictions can be verified.

(1) The predicted absence of a Korringa term in the relaxation rate at nonactinide/rare-earth nuclei, even in severely gapless heavy-fermion superconductors. This requires careful measurements of the relaxation rate and specific heat on the same samples.

(2) The appearance of a *sharp* gap in the f-spin excitation spectrum, which should manifest itself by an exponential reduction in the NMR linewidth of the actinide or rare-earth nuclei at low temperatures. This feature should make it possible to resolve the NMR line at the heavy-fermion site in the superconducting phase.

Another area of fruitful investigation concerns the field dependence of the proximity effect. Negative proximity effects have been observed between UBe_{13} and Ta superconductors.[54] If the symmetry of heavy-fermion superconductors has a different temporal parity, then we expect the application of a magnetic field to enhance the coupling between the two order parameters, leading to a strong reduction of the negative proximity effect in a field, and a strong field dependence of the Josephson current.

In conclusion, we have presented a stable realization of odd-frequency triplet pairing in a Kondo lattice model for heavy fermions. Under rather general conditions, the odd-frequency state that forms has a gapless singlet mode of quasiparticles. Spin and charge coherence factors for these quasiparticles grow linearly in their energy. Our pairing hypothesis provides an alternative explanation of various power laws in heavy fermions in terms of a vanishing of coherence factors at the Fermi energy, rather than a vanishing of the density of states. We have conjectured that this may explain the absence of a Korringa law in the NMR relaxation rate, even when the superconductor is highly gapless. Odd-frequency triplet superconductivity appears to be able to coexist with magnetism, and in our simple toy model, ferromagnetic order coexists with the pairing. We think our results are encouraging enough to prompt efforts to develop a description of odd-frequency pairing within more general models, and to consider seriously the possibility that this provides a viable alternative to the *d*-wave pairing hypothesis in heavy-fermion superconductors.

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APPENDIX A: MAJORANA REPRESENTATION OF SPINS

In this section, we present a derivation of the Majorana representation that provides a link with the Abrikosov fermion representation and illustrates how the constraint is avoided by the uniform replication of the spin Hilbert space. We begin by noting that for any two-component electron spinor there are two operators of interest: the "spin"

$$\mathbf{s}=f^{\dagger}_{\alpha}\left[\frac{\boldsymbol{\sigma}}{2}\right]_{\alpha\beta}f_{\beta} \tag{A1}$$

and the "isospin"

$$\boldsymbol{\tau}=\tilde{f}^{\dagger}_{\alpha}\left[\frac{\boldsymbol{\sigma}}{2}\right]_{\alpha\beta}\tilde{f}_{\beta}\ , \tag{A2}$$

where we have introduced the Nambu spinor

$$\tilde{f}=\begin{bmatrix} f_{\uparrow} \\ f^{\dagger}_{\downarrow}\end{bmatrix}\ . \tag{A3}$$

These operators are independent $[s_a,\tau_b]=0$ and each satisfy an SU(2) algebra

$$[s_i,s_j]=i\epsilon^{ijk}s_k,\quad [\tau_i,\tau_j]=i\epsilon^{ijk}\tau_k\ . \tag{A4}$$

In the subspace where the spin is finite, the isospin is zero, and vice versa. The *sum* of both operators

$$\mathbf{S}=\mathbf{s}+\boldsymbol{\tau} \tag{A5}$$

satisfies an SU(2) algebra, and is either equal to the "spin" or "isospin," depending on which component of the Fock space is projected. For any interacting system of electrons containing N local moments, we may write the partition function as a constrained trace

$$Z=\mathrm{Tr}\left[\prod_j P_j^{q_j}\exp(-\beta H[\mathbf{S}_j])\right]\quad (q_j=s,\tau) \tag{A6}$$

with

$$\mathbf{S}_j=f^{\dagger}_{j\alpha}\left[\frac{\boldsymbol{\sigma}}{2}\right]_{\alpha\beta}f_{j\beta}+\tilde{f}^{\dagger}_{j\alpha}\left[\frac{\boldsymbol{\sigma}}{2}\right]_{\alpha\beta}\tilde{f}_{j\beta}\ , \tag{A7}$$

where the projection operator $P_j^{q_j}$ projects the "spin" or "isospin" component of the Fock space at site j

$$P_j^{\tau}=(n_j-1)^2,\quad P_j^{s}=(n_{j\uparrow}-n_{j\downarrow})^2,\quad P_j^s+P_j^{\tau}=1\ . \tag{A8}$$

There are then 2^N ways of choosing the projection operators: each choice projects a replica of the spin Hilbert space with precisely the same partition function. Summing over all replicas we can write

$$Z=\frac{1}{2^N}\sum_{q_j=s,\tau}\mathrm{Tr}\left[\prod_j P_j^{q_j}\exp(-\beta H[\mathbf{S}_j])\right]\ . \tag{A9}$$

The sum over all 2^N projectors is the identity operator

$$\sum_{q_j=s,\tau}\prod_j P_j^{q_j}=\prod_j[P_j^s+P_j^{\tau}]=1 \tag{A10}$$

and hence the replicated partition function can be written as an *unconstrained* trace, with each local moment represented as a sum of the Pauli spin and isospin:

$$Z=\frac{1}{2^N}\mathrm{Tr}[\exp(-\beta H[\mathbf{S}_j])]\ . \tag{A11}$$

We now demonstrate that the combined operator $\mathbf{S}=\mathbf{s}+\boldsymbol{\tau}$ depends only on three Majorana components of the f electron. Suppose we decompose the complex Fermi operators into their real and imaginary Majorana components as follows:

$$f_j=\frac{1}{\sqrt{2}}(\eta_o+i\boldsymbol{\sigma}\cdot\boldsymbol{\eta})z_o\ ,\quad z_o=\begin{bmatrix}0\\ i\end{bmatrix}\ . \tag{A12}$$

In terms of these components, the "spin" and "isospin" operators are

$$\begin{aligned} s_j^i&=\frac{i}{2}[\eta_j^0\eta_j^i-\tfrac{1}{2}\epsilon_{ilm}\eta_j^l\eta_j^m]\ ,\\ \tau_j^i&=-\frac{i}{2}[\eta_j^0\eta_j^i+\tfrac{1}{2}\epsilon_{ilm}\eta_j^l\eta_j^m]\ . \end{aligned} \tag{A13}$$

The sum of these two is then

$$s_j^i+\tau_j^i=-\frac{i}{2}\epsilon^{ilm}\eta_j^l\eta_j^m\ , \tag{A14}$$

which is precisely our Majorana representation. With this choice of z, the zeroth component of the Majorana fermions at each site does not enter into the Hamiltonian. This component can therefore be explicitly traced out of the partition function. Formally, this may be done by pairing the zeroth Majorana fermions throughout the lattice

$$a_\lambda=\frac{1}{\sqrt{2}}(\eta^0_{i_\lambda}-i\eta^0_{j_\lambda})\quad (\lambda=1,2,\ldots,N/2)\ , \tag{A15}$$

where each site l belongs to one pair: $l \in \{(i_\lambda, j_\lambda), \lambda = 1, N\}$. The set of $N/2$ *complex* fermions are independent and form a completely decoupled zero energy Fock space of dimension $2^{N/2}$. Hence

$$Z = \frac{1}{2^{N/2}} \mathrm{Tr}\left\{ \exp\left[-\beta H \left[\mathbf{S}_j \to -\frac{i}{2} \boldsymbol{\eta}_j \times \boldsymbol{\eta}_j \right] \right] \right\} , \quad \text{(A16)}$$

where the remaining unconstrained trace is over the $l = 1,2,3$ components of each Majorana fermion, and the other real electron states of the system.

The overcompleteness of our representation is closely related to a residual discrete local Z_2 symmetry of the Majorana spin representation under the transformation

$$\boldsymbol{\eta}_j \to -\boldsymbol{\eta}_j \ . \quad \text{(A17)}$$

In this respect, the Majorana representation is similar to the pseudofermion representation. However, in this case, the canonical and grand-canonical ensembles have precisely the same partition function, up to a simple normalization factor. In the pseudofermion representation, the Gibbs partition function for each conserved subspace is not constant (for if $n_j = 0$ or $n_j = 2$ there is no spin at site j), and the projection of the unwanted spaces is an unavoidable necessity.

Majorana fermions are easily treated in a momentum space representation. The Fourier-transformed operators

$$\boldsymbol{\eta}_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} \boldsymbol{\eta}_i \ . \quad \text{(A18)}$$

Since the original Majorana fermions are real $\eta_j^a = \eta_j^{a\dagger}$, their complex Fourier transforms satisfy $\eta_{\mathbf{k}}^a = \eta_{-\mathbf{k}}^{a\dagger}$, forming a set of independent complex fermions that span half of the Brillouin zone:

$$\{\eta_{\mathbf{k}}^a, \eta_{\mathbf{k}'}^{b\dagger}\} = \delta_{a,b}\delta_{\mathbf{k},\mathbf{k}'} ,$$
$$\mathbf{k},\mathbf{k}' \in \text{half the Brillouin zone} . \quad \text{(A19)}$$

The inverse transformation can be written

$$\boldsymbol{\eta}_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in 1/2\ \mathrm{BZ}} \{ \boldsymbol{\eta}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_j} + \boldsymbol{\eta}_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{R}_j} \} \ . \quad \text{(A20)}$$

The corresponding Lagrangian for the Majorana is then

$$\mathcal{L} = \sum_{\mathbf{k}\in 1/2\ \mathrm{BZ}} \boldsymbol{\eta}_{\mathbf{k}}^\dagger \cdot \partial_\tau \boldsymbol{\eta}_{\mathbf{k}} + \mathcal{H} \quad \text{(A21)}$$

or in terms of the original site representation

$$\mathcal{L} = \frac{1}{2} \sum_i \boldsymbol{\eta}_i \cdot \partial_\tau \boldsymbol{\eta}_i + \mathcal{H} \ . \quad \text{(A22)}$$

Note that for each momentum $\mathbf{k}$, we can choose either $\eta_{\mathbf{k}}$ or $\eta_{-\mathbf{k}} = \eta_{\mathbf{k}}^\dagger$ as the independent destruction operator. This has an important consequence for broken symmetry solutions, for there are $2^{N/2}$ equivalent ways of making the choice of the vacuum state: by making one particular choice, the normalization constant in front of the partition function is absorbed.

APPENDIX B: SOME SIMPLE EXAMPLES

In this appendix, we illustrate the use of the Majorana fermion representation of spin $\frac{1}{2}$, by means of some specific examples. Consider first the Heisenberg model for two spins $\frac{1}{2}$ (where we take the exchange coupling to be 1), written in terms of the Majorana fermions

$$H = \mathbf{S}_1 \cdot \mathbf{S}_2 = \tfrac{1}{2}[(\boldsymbol{\eta}_1 \cdot \boldsymbol{\eta}_2)^2 + \tfrac{3}{4}] \ . \quad \text{(B1)}$$

One can now define three complex fermions, by taking appropriate linear combinations of the six Majorana fermions

$$\mathbf{f} \equiv \frac{1}{\sqrt{2}} (\boldsymbol{\eta}_1 - i\boldsymbol{\eta}_2) ,$$
$$\mathbf{f}^\dagger \equiv \frac{1}{\sqrt{2}} (\boldsymbol{\eta}_1 + i\boldsymbol{\eta}_2) \ . \quad \text{(B2)}$$

These operators satisfy the usual fermionic anticommutation algebra

$$\{f^i, f^{j\dagger}\} = \delta_{ij} \quad (i,j = 1,3) \quad \text{(B3)}$$

and act on a Hilbert space of dimension $2^3 = 8$. As pointed out in the first section, the dimensionality of the original space has been increased by a factor of $2^{(\mathcal{N}/2)} = 2$, where $\mathcal{N} = 2$ is the number of spins.

By using

$$-i\boldsymbol{\eta}_1 \cdot \boldsymbol{\eta}_2 = \mathbf{f}^\dagger \cdot \mathbf{f} - \tfrac{3}{2} , \quad \text{(B4)}$$

one can now write the Hamiltonian in terms of the f operators

$$H = \tfrac{3}{8} - \tfrac{1}{2}(\mathbf{f}^\dagger \cdot \mathbf{f} - \tfrac{3}{2})^2 \ . \quad \text{(B5)}$$

The spectrum can now be easily worked out

$$E_0 = -\tfrac{3}{4} ,$$
$$E_1 = \tfrac{1}{4} \ . \quad \text{(B6)}$$

The first level is doubly degenerate and the second one is sixfold degenerate. The exact eigenenergies are correctly obtained, as expected. Besides, the singlet ground state and the triplet excited state are replicated by the same factor of 2. This additional degeneracy can be traced back to the invariance of the Majorana representation with respect to the Z_2 transformations $\boldsymbol{\eta}_i \to -\boldsymbol{\eta}_i$, which is reflected in a particle-hole symmetry of the Hamiltonian $\mathbf{f} \to \mathbf{f}^\dagger$.

A mean-field treatment of this model can be performed by the following decoupling procedure:

$$H_{\mathrm{MF}} = \tfrac{3}{8} + iV(\boldsymbol{\eta}_1 \cdot \boldsymbol{\eta}_2) + \frac{V^2}{2}$$
$$= \tfrac{3}{8} - V(\mathbf{f}^\dagger \cdot \mathbf{f} - \tfrac{3}{2}) + \frac{V^2}{2} \ . \quad \text{(B7)}$$

A static order parameter V breaks the aforementioned Z_2 symmetry and there are two stable solutions related to each other by the transformation

$$V \to -V, \quad \mathbf{f} \to \mathbf{f}^\dagger \ . \quad \text{(B8)}$$

If V is positive, the ground state corresponds to $\mathbf{f}^\dagger\cdot\mathbf{f}-\frac{3}{2}=V=\frac{3}{2}$ and its energy is $-\frac{3}{4}$, which is the exact value.

Consider now the one-dimensional XY model, which can be solved exactly through a mapping to a free-fermion model. This mapping is conventionally performed by means of a Jordan-Wigner transformation. It will now be shown that an analogous mapping can be achieved through the Majorana representation of spins.

The 1D XY model Hamiltonian is given by

$$H_{XY}=\sum_{i=1}^{\mathcal{N}}(S_x^iS_x^{i+1}+S_y^iS_y^{i+1})=\frac{1}{2}\sum_{i=1}^{\mathcal{N}}(S_+^iS_-^{i+1}+S_-^iS_+^{i+1})\ . \tag{B9}$$

In terms of the Majorana fermions, one can write

$$S_+^i\equiv S_x^i+iS_y^i=\eta_3^i(\eta_1^i+i\eta_2^i)\ ,\qquad S_-^i\equiv S_x^i-iS_y^i=(\eta_1^i-i\eta_2^i)\eta_3^i\ . \tag{B10}$$

At each site one can define a complex fermion

$$c^i\equiv\frac{1}{\sqrt{2}}(\eta_1-i\eta_2)\ ,\qquad c^{i\dagger}\equiv\frac{1}{\sqrt{2}}(\eta_1+i\eta_2)\ , \tag{B11}$$

satisfying

$$\{c^i,c^{j\dagger}\}=\delta_{ij}\quad\{c^i,\eta_3^j\}=0\quad\{c^{i\dagger},\eta_3^j\}=0\ . \tag{B12}$$

The Hamiltonian can now be written as

$$H_{XY}=\sum_{i=1}^{\mathcal{N}}(c^{i\dagger}\eta_3^i\eta_3^{i+1}c^{i+1}+c^i\eta_3^i\eta_3^{i+1}c^{i+1\dagger})\ . \tag{B13}$$

Let U^i be an operator acting on site i

$$U^i\equiv P_0^i+\sqrt{2}\eta_3^iP_1^i\ , \tag{B14}$$

where

$$P_0^i\equiv 1-c^{i\dagger}c^i,\quad P_1^i\equiv c^{i\dagger}c^i\ , \tag{B15}$$

are projectors onto the vacant and occupied states of site i. The operator U^i is both Hermitian and unitary

$$U^{i\dagger}=P_0^i+\sqrt{2}P_1^i\eta_3^i=U^i\ ,\qquad U^iU^{i\dagger}=U^{i\dagger}U^i=P_0^{i2}+2\eta_3^{i2}P_1^{i2}=P_0^i+P_1^i=1\ . \tag{B16}$$

One can now easily prove that

$$U^i(\eta_3^ic^{i\dagger})U^{i\dagger}=\frac{c^{i\dagger}}{\sqrt{2}}\ ,\qquad U^i(c^i\eta_3^i)U^{i\dagger}=\frac{c^i}{\sqrt{2}}\ . \tag{B17}$$

The canonical transformation generated by U^i transforms away the third Majorana component.

Let U be the ordered product

$$U\equiv\prod_{i=1}^{\mathcal{N}}U^i\ . \tag{B18}$$

Under the action of U, the transformed operator now acquires a nonlocal phase factor

$$U(\eta_3^ic^{i\dagger})U^\dagger=\prod_{j=1}^{i}U^j(\eta_3^ic^{i\dagger})\prod_{k=i}^{1}U^k=\prod_{j=1}^{i-1}U^j\left[\frac{c^{i\dagger}}{\sqrt{2}}\right]\prod_{k=i-1}^{1}U^k=(-1)^{\sum_{j=1}^{i-1}n_j}\left[\frac{c^{i\dagger}}{\sqrt{2}}\right]\ , \tag{B19}$$

where $n_j=c^{j\dagger}c^j$, and, in the last step, use has been made of

$$U^j(c^{i\dagger})U^j=c^{i\dagger}(P_0^j-\sqrt{2}\eta_3^jP_1^j)(P_0^j+\sqrt{2}\eta_3^jP_1^j)=c^{i\dagger}(-1)^{n_j}\quad(i\neq j)\ . \tag{B20}$$

Using relation (B19) and its complex conjugate, one can transform the Hamiltonian into

$$\begin{aligned}H'_{XY}&=UH_{XY}U^\dagger\\&=\sum_{i=1}^{\mathcal{N}}(Uc^{i\dagger}\eta_3^iU^\dagger U\eta_3^{i+1}c^{i+1}U^\dagger+Uc^i\eta_3^iU^\dagger U\eta_3^{i+1}c^{i+1\dagger}U^\dagger)\\&=\frac{1}{2}\sum_{i=1}^{\mathcal{N}}(c^{i\dagger}c^{i+1}(-1)^{n_i}+c^ic^{i+1\dagger}(-1)^{n_i})\\&=\frac{1}{2}\sum_{i=1}^{\mathcal{N}}(c^{i\dagger}c^{i+1}-c^ic^{i+1\dagger})\ ,\end{aligned} \tag{B21}$$

which is the usual free-fermion expression obtained by the Jordan-Wigner transformation. The third Majorana components have been transformed out of the problem. Tracing over these variables will cancel out the overall factor of $2^{\mathcal{N}/2}$ and one is left with a free-fermion theory.

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