Plasma oscillations in heavy-fermion materials

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We calculate the dielectric function of the lattice Anderson model via an auxiliary-boson large-N method suitably generalized to include the effects of the long-range part of the Coulomb interaction. We show that the model exhibits a low-lying plasma oscillation at a frequency ω^* on the order of the Kondo temperature of the model, in addition to the usual high-frequency plasma oscillation. We also analyze the Anderson model without the long-range Coulomb interaction, computing the Landau parameter F_{0s}, and showing that the model has a zero-sound mode whose velocity we compute. We derive the version of the f sum rule applicable to our model and show that our results satisfy it.

Heavy-electron metals are a class of compounds involving rare-earth or actinide elements which have recently been much studied[1,2] because at low temperatures their properties are, crudely speaking, those of a Fermi liquid of mass $m^* \sim 10^2 m$ (m is the usual electron mass) and Fermi temperature $T^* \sim 10$–100 K. Here we report results of a theoretical study of the small-q limit of the dielectric function $\epsilon(q,\omega)$. Our principle result is that heavy-electron metals should have a plasmon mode at the renormalized plasma frequency $\omega^* \cong T^*$. The plasmon has low spectral weight, making an order m/m^* contribution to the f sum rule, and is likely to be damped, but perhaps ought to be observable in reflectivity or other measurements. We also relate our results to a previous calculation[3] of the optical conductivity $\sigma(\omega)$, and comment on the implication of our results for the physical interpretation of the heavy-fermion compounds.

As a model for the low-temperature behavior of heavy-electron materials we use the auxiliary-boson (or "slave-boson") large-N version of the lattice Anderson model. The Anderson model is believed[2] to represent the essential physics of heavy-fermion materials. The slave-boson, large-N version was devised for the single-impurity Anderson model[4-6] and has been also used to study various aspects of the lattice problem.[3,7-10] For a comparison of this with other methods, see Ref. 2.

The Anderson model describes a structureless band of conduction electrons (operator $c_{k\sigma}$, energy ε_k) hybridizing via a hybridization matrix element V (conventionally assumed to be structureless), with a dispersionless band of f electrons at an energy E_0, and subject to the constraint that the number of f electrons on site i, $n_{fi} \leq 1$. We measure all energies with respect to the chemical potential (taken to be zero) and we are interested in the Kondo limit in which $-E_0/\rho_0 V^2 \gg 1$. ρ_0 is the c-electron density of states evaluated at $\varepsilon_k = 0$. We assume $T = 0$ throughout.

The Anderson model as conventionally formulated does not include the (physically necessary) long-range part of the Coulomb interaction. We therefore add to it a term of the form

$$H_{\text{Coul}} \sim \sum_{q < q_c} \frac{4\pi e^2}{q^2} n_q n_{-q} \ ,$$

where n_q is the Fourier transform of the density $n_i = n_{ci} + n_{fi}$. We note that the short-range part of the Coulomb interaction between the f electrons is already included in the Anderson model, where it produces the "infinite-U" repulsion leading to the constraint $n_{fi} \leq 1$. However, the long-range part of this interaction is not included, as can be seen from a *Gedankenexperiment* in which a few f electrons are moved from one end of the lattice to the other, with everything else held fixed. The sum on q in H_{Coul} must be cut off at $q = q_c \ll k_F$ to avoid double counting. In this Rapid Communication we are concerned only with asymptotically-long-wavelength properties, and will never have to specify q_c.

The inequality constraint on n_f makes the model difficult to attack by conventional methods. In the slave-boson method one introduces a new boson field b_i representing an empty set of f orbitals on site i, rewrites the hybridization $(Vc_i^\dagger f_i b_i^\dagger + \text{H.c.})$ and enforces the constraint $n_{fi} + n_{bi} = 1$ via a Lagrange multiplier field λ. To use the $1/N$ expansion one assumes both c and f electrons are characterized by a N-fold–degenerate "spin" quantum number m, conserved in hybridization and c-electron propagation, and one rewrites the constraint as $n_{fi} + n_{bi} = q_0 N$, where q_0 is regarded formally as independent of N. (To recover the original Anderson model one sets $q_0 \to 1/N$ at the end of any calculation.[3]) Next, one splits the boson operators into static and fluctuating parts. Retaining only the static parts leads to a mean-field theory of electrons moving in a renormalized band structure in

which a dispersionless band of f quasiparticles[3] at energy $T^* > 0$ hybridizes via a renormalized hybridization $\sigma_0 \ll V$ with the c-electron band. Corrections to the mean-field theory come from Coulomb interactions and interactions between the electrons and the fluctuating parts of the boson fields. To study these corrections we use the radial gauge formulation,[5] but we write the electrons in terms of the operators d_i which diagonalize the mean-field theory, and we take the small-q limit in the interaction terms. The model is then specified by the Lagrangian $L = L_F + L_B + L_I + L_{Coul} + L_{rest}$, where

$$L_F = \sum_{i,k,m} d_{ikm}^\dagger [\partial_\tau + \varepsilon_i(k)] d_{ikm} , \tag{1a}$$

$$L_B = \frac{N}{2V^2} \sum_q \sigma_q (T^* - E_0)\sigma_q + 2i\sigma_0 \sigma_q \lambda_{-q} , \tag{1b}$$

$$L_I = \sum_{k,q,m} d_{1,k+q,m}^\dagger d_{1km} \left[\frac{2\sigma_0}{E_k}\sigma_q + i\lambda_q \right]$$
$$+ (d_{2km}^\dagger d_{1,k+q,m} + \text{H.c.}) \left[\frac{\varepsilon_k - \varepsilon_f}{E_k}\sigma_q - \frac{i\sigma_0}{E_k}\lambda_q \right] , \tag{1c}$$

$$L_{Coul} = \sum_{q(<q_c)} \frac{4\pi e^2}{Nq^2} n_q n_{-q} , \tag{1d}$$

where the $d_{1(2)km}$ and $\varepsilon_{1(2)k}(k)$ are the operators and energies for the lower and upper bands of the renormalized band structure; one has

$$\varepsilon_{1(2)}(k) = \tfrac{1}{2}[(\varepsilon_k + T^*) - (+) E_k]$$

and

$$E_k = \sqrt{(\varepsilon_k - T^*)^2 + 4\sigma_0^2} .$$

We have assumed the Fermi level lies in the lower band. The d_{ki} are related to the c and f operators via

$$d_{ki} = \cos\theta_{ki} c_{ki} + \sin\theta_{ki} f_{ki} ,$$

where

$$\tan\theta_{ki} = [\varepsilon_i(k) - \varepsilon_k]/\sigma_0 = \sigma_0/[\varepsilon_i(k) - T^*] .$$

The mean-field parameters σ_0 and T^*, to leading order in $1/N$, and q_0 are given by[3] $T^* = D\exp(E_0/\rho_0 V^2)$, $\sigma_0^2 = q_0 V^2 (1 - n_f)$, and $n_f = (1 + T^*/\rho_0 V^2)^{-1}$. Here D is an energy of the order of the distance of the bottom of the c-electron band from the chemical potential. The density of states at the Fermi surface $\varepsilon_1(k) = 0$ is $(m^*/m) \times (k_F^2/2\pi^2)(dk/d\varepsilon_k)$, where $m^*/m = \sigma_0^2/(T^*)^2 = \varepsilon_{k_F}^2/\sigma_0^2$. The band structure defined by L_F is thus very flat at k_F; its excitations are heavy fermions of velocity $v^* = d\varepsilon_1(k_F)/dk$. The band structure has a direct gap of magnitude $2\sigma_0$ centered at $\varepsilon_k = T^*$.

The operators σ_q and λ_q are related to the fluctuating part of the original Bose operators. In terms of the operators d_i, the density operator is

$$n_q = \sum_{k,m} d_{1,k+q,m}^\dagger d_{1km} + \mathbf{p}_k \cdot \mathbf{q}(d_{2,k+q,m}^\dagger d_{1km} + \text{H.c.}) , \tag{2}$$

$\mathbf{p}_k = (\sigma_0/E_k^2)(d\varepsilon_k/d\mathbf{k})$ is the dipole operator which gives

rise to interband transitions.

The factor of N in L_{Coul} arises because we consider a model with ~ 1 electron per spin channel.

The expressions above are correct only up to terms of relative order $(q/k_F)^2$. The terms in L_{rest}, which we have not explicitly written, include a three-boson interaction (which does not contribute to the order to which we work) with the terms which fix the mean-field parameters, and the terms involving band-2 operators which do not contribute at $T = 0$.

From Eqs. (1)–(4) one may easily compute the density-density correlation function $\chi(q,\omega)$ by standard diagrammatic techniques. Details of a similar calculation are given in Ref. 10. To leading order in $1/N$ the only diagrams which contribute are shown in Fig. 1. They have the familiar random-phase-approximation (RPA) form of polarization bubbles connected by interaction lines, which in this case may be either boson propagators [from Eq. (1b)] or the Coulomb interaction. The polarization bubbles may be of inter- or intra-band type. Note that the density operator (and thus the Coulomb interaction) couples to an interband bubble via a vector vertex, but the boson propagator couples to an interband bubble via a scalar vertex. Summing the diagrams we find at small q,

$$\chi(q,\omega) = -\frac{\Pi(q,\omega) + \Pi_{12}^0(q,\omega)}{1 + (4\pi e^2/q^2 N)[\Pi(q,\omega) + \Pi_{12}^0(q,\omega)]} . \tag{3}$$

Here Π_{12}^0 is the interband density polarization bubble,

$$\Pi_{12}^0(q,\omega) = -N \sum_{k(<k_F)} (\mathbf{p}_k \cdot \mathbf{q})^2$$
$$\times \left[\frac{1}{\omega - E_k + i\delta} + \frac{1}{-\omega - E_k - i\delta} \right] , \tag{4}$$

and $\Pi(q,\omega)$ is the intraband density polarization bubble, which includes the effects of electron–slave-boson interactions. One finds

$$\Pi(q,\omega) = \Pi_0(q,\omega)/1 + \Gamma_B(\omega)\Pi_0(q,\omega) , \tag{5}$$

where Π_0 is the bare intraband polarization bubble;

$$\Pi_0(q,\omega) = -N \sum_k \frac{f(\varepsilon_1(k)) - f(\varepsilon_1(k+q))}{\omega + \varepsilon_1(k) - \varepsilon_1(k+q) + i\delta} . \tag{6}$$

Γ_B is the effective boson-mediated interaction between two band-1 quasiparticles with $k \cong k_F$. It is made up of

$$\chi(q,\omega) = \quad\bigcirc\!\!\!\!\bigcirc \quad + \quad \bigcirc\!\!\!\!\bigcirc ---\bigcirc\!\!\!\!\bigcirc \quad + \cdots$$

FIG. 1. Diagrams for density-density correlation function, to leading order in $1/N$. The heavy dots denote density vertices. The solid lines with arrows represent electron Green's functions obtained from the inverse of L_F, Eq. (2a) in the text. The dashed line represents either bare boson propagators obtained from inverting L_B, Eq. (2b) in the text, or the Coulomb interaction $4\pi e^2/q^2 N$. The vertices at which boson or Coulomb lines join fermion lines are obtained from L_I, Eq. (2c) and L_c, Eq. (2d), respectively.

bare boson propagators appropriately dressed by inter-band bubbles. Γ_B is a function of ω/σ_0 and we shall require only its $\omega \to 0$ limit, which we find to be $\Gamma_B(0) = (m^*/m\rho)$.

Equation (3) is the central result of this paper. To understand it, we first study the model without long-range electric fields by setting $e^2 = 0$. Equation (3) then becomes $\chi = \Pi + \Pi_{12}^0$. The term in Π_{12}^0, which is explicitly of order q^2, gives the contribution to χ from interband transitions. The term in Π gives the intraband contribution, which is altered from the "noninteracting" value Π_0 by the electron-boson interactions. By using Eqs. (3)–(6) we find $\lim_{q \to 0} \chi(q,0) = \rho(1/1 + \rho \Gamma_B)$. We therefore identify $\rho \Gamma_B(\omega = 0)$ with the Landau parameter $F_{0s} = m^*/m \gg 1$. All other Landau F parameters are of order $1/N$.[3,8] Note also that χ has a pole at $\omega^2 = c^2 q^2$, with $c^2 = (F_{0s}/3)v^{*2}$; this is the familiar zero-sound mode of a neutral Fermi liquid with $F_{0s} \gg 1$. The Fermi liquid under consideration stems from the hybridization of two bands, one of which is dispersionless. The model is therefore not Galilean invariant. In a Galilean-invariant Fermi liquid with $m^*/m \gg 1$, the expression for the zero-sound velocity would necessarily involve also $F_{1s} = 3[(m^*/m) - 1]$.

Consider now the spectral weight of density-fluctuation excitations, $S(q,\omega) = (1/\pi) \text{Im} \chi(q,\omega)$. $S(q,\omega)$ satisfies the f sum rule[11]

$$\int_0^\infty d\omega \, \omega S(q,\omega) = n_{tot} q^2/2m \ ,$$

where n_{tot} is the total number of electrons and m is the electron mass. The Anderson model, however, is an effective Hamiltonian presumed to describe the physics of heavy-fermion materials at energies less than the conduction-electron bandwidth, which is of order D. In particular, higher-excited states of the f electrons, which presumably form bands at energies $\gtrsim D$ above the Fermi surface, are not included. These higher bands will contribute, at high frequencies, to the f sum rule; therefore, the S derived from Eq. (3) does not satisfy the full f sum rule. However, by applying the standard derivation[11] of the f sum rule to the Anderson model we have derived a partial f sum rule

$$\int_0^\infty d\omega \, \omega S(q,\omega) = n_c q^2/2m \ . \tag{7}$$

Here n_c is the number of conduction electrons. (We assume unit volume.) If one assumes $\varepsilon_k = k^2/2m - \mu$, then $n_c = N k_h^3/6\pi^2$ where $k_h = \sqrt{2m\mu}$. We expect that the difference $(n - n_c)q^2/2m$ between (7) and the full f sum rule is made up by the previously mentioned interband contributions to $S(q,\omega)$ at $\omega \gtrsim D$.

Now using Eq. (3) one may easily check that (7) is satisfied at small q. In the case $e^2 = 0$ there are three contributions. One comes from the particle-hole continuum near the Fermi surface, $\omega < v^*q$, and contributes a term of order $n_c q^2/F_{0s}^2 m^*$ to the right-hand side of (7). Thus the low-lying quasiparticle density fluctuations have negligible spectral weights. The second contribution comes from the zero-sound mode; it contributes $nq^2/2m^*$, where in a model with a spherical Fermi surface, $n = N k_F^3/6\pi^2$. The third contribution comes from the interband transitions at frequencies $\omega \gtrsim 2\sigma_0$ contained in Π_{12}^0, yielding $n_c q^2/2m - (nq^2/2m^*)$.

It is now accepted that the low-energy excitations about the $T = 0$ ground state of the lattice Anderson model are those of a Fermi liquid of large effective mass m^*.[2,3,8,12] It has also been asserted that the effective density of particles in the Fermi liquid is $n(m/m^*)$.[12] One may interpret the results of the present paper as supporting this assertion, because the "Fermi-liquid" contributions (from the intraband particle-hole continuum and the zero-sound mode) to $S(q,\omega)$ contribute only $n(m/m^*)q^2/2m$ to the total spectral weight required by the f sum rule. However, it is also argued in Ref. 12 that $n(m/m^*) \sim (1 - n_f)$, so that heavy fermions are to be interpreted as holes in the f band. This assertion is not supported by the present model because n_f and m^*/m are separate parameters of the model and can be independently varied by appropriate variations of the bare parameters E_0 and V.

We now consider the physically relevant model, in which long-range Coulomb forces are present. For charged systems the relevant quantity is the dielectric function, $\epsilon(q,\omega)$, which may be computed either directly from the diagrams for the dressed Coulomb interaction or from the identity

$$\epsilon^{-1}(q,\omega) = 1 + (4\pi e^2/q^2)\chi(q,\omega) \ .$$

By either method one finds

$$\epsilon(q,\omega) = 1 + \frac{4\pi e^2}{q^2}[\Pi(q,\omega) + \Pi_{12}^0(q,\omega)] \ . \tag{8}$$

In the static limit, $\omega = 0$, $\Pi(q,\omega) \to \rho/1 + F_{0s}$, while Π_{12}^0 tends to the value $(q^2/4\pi e^2)(\omega_{pc}^2/6\sigma_0^2)$, where $\omega_{pc}^2 = 4\pi n_c e^2/m$. Thus

$$\epsilon(q,0) = \epsilon_0 + \frac{4\pi e^2}{q^2}\left[\frac{\rho}{1 + F_{0s}}\right] \ .$$

Here $\epsilon_0 = 1 + \omega_{pc}^2/6\sigma_0^2$. In physical terms ϵ_0 represents a reduction in the Coulomb interaction between band-1 quasiparticles due to polarization of the "light" c-electron degrees of freedom. Because $F_{0s} = m^*/m$, the Thomas-Fermi screening length is not renormalized from a value characteristic of a conventional light-electron system.

The frequency-dependent conductivity $\sigma(\omega)$ is related to the dielectric function by

$$\lim_{q \to 0} \epsilon(q,\omega) = 1 + 4\pi i \sigma(\omega)/\omega \ .$$

The results presented here for $\epsilon(q,\omega)$ agree with results previously calculated[3] for $\sigma(\omega)$ in the limit $N \to \infty$, $\tau \to \infty$ (τ is the impurity scattering time defined in Ref. 3).

Zeros of $\epsilon(q,\omega)$ correspond to plasma oscillations of the system. There are two in this model, at $\omega = \omega_{high}$ and $\omega = \omega^*$, where, using Eqs. (3)–(5) and (8),

$$\omega_{high}^2 = \omega_{pc}^2 - O(m/m^*) \ , \tag{9a}$$

$$\omega^{*2} = 6(1 + n_f/n_c)T^{*2} \ . \tag{9b}$$

The high-frequency plasma oscillation occurs at approximately the plasma frequency of the c electrons alone. This is to be expected: Heavy-fermion behavior is essentially a low-frequency and -temperature phenomenon, which should not affect high-frequency phenomena such

as the plasma oscillation.

The low-frequency oscillation may be thought of as a heavy fermion plasma mode. It is reduced from a typical plasma frequency $\omega_p^2 = 4\pi e^2 n/m$ by two effects: (i) the mass enhancement (m^*/m) and (ii) the reduction of the effective Coulomb interaction between two band-1 quasiparticles which is given by ϵ_0. The low-frequency plasma oscillation may be thought of as the zero-sound oscillation of the neutral system, pushed up to a finite frequency by the long range of the Coulomb interaction. It has spectral weight $nq^2/2m^*$ as does the zero-sound mode.

The form for ϵ is precisely what would be expected for a metal which happened to have the "mean-field" band structure described by Eq. (1a).[13] However, the mean-field solution is valid only for $T \ll T^*$; for larger T a picture in which c electrons are incoherently scattered by spin fluctuations is more appropriate. Our theory applies only for very low temperatures, but we suspect that Reϵ would not have a low-lying zero crossing for temperatures comparable to or greater than T^*.

Zeroes of ϵ correspond to poles in $\mathcal{X}$. By using Eq. (3) with for the charged case one easily verifies that to leading order in q^2 the only contributions to (7) come from the two plasmon poles. The plasmon at ω^* contributes $nq^2/2m^*$; the plasmon at ω_{high} contributes $n_c q^2/2m - nq^2/2m^*$. Thus the low-lying plasmon has spectral weight $nq^2/2m^*$ as did the zero sound mode of the neutral system. Note that Re$\epsilon(q,\omega)$ also vanishes at a value $\omega = \omega_0 \gtrsim 2\sigma_0$. However, at $\omega = \omega_0$, Imϵ is large because of interband transitions. This zero of Reϵ therefore corresponds to a heavily damped oscillation, and not to a distinguishable mode of the system. The other two plasma modes are undamped, to leading order in $1/N$.

To summarize, we have calculated the dielectric function for the Anderson lattice to leading order in $1/N$ using the slave-boson method. We have included the long-range part of the Coulomb interaction. We have shown that the model exhibits a low-frequency plasma oscillation at a frequency $\omega^* \sim T^*$, where T^* is the characteristic or Kondo temperature of the model, as well as the usual high frequency plasmon.

In conclusion, we discuss the observability of the low-lying plasmon in real heavy-fermion materials. We first note that the characteristic energy scale is set by T^*, the Fermi temperature of the heavy fermions. T^* determines the coefficient of the linear term in the low-temperature specific heat and the T^2 term in the resistivity.[3] T^* determines the heavy-fermion plasma frequency $(n_f/n_c$ is of the order 1), and our calculation only applies for temperatures small compared to T^*. In the very-low-temperature regime where our calculation is valid, the low-lying plasmon is undamped to leading order in $1/N$. However, the system is not Galilean-invariant; therefore $1/N$ effects involving inelastic scattering of electrons off of slave-boson fluctuations could, in a system in which N is not large, lead to a large value of Im$\epsilon(q,\omega)$ for $\omega \sim T^*$. This would substantially broaden the low-lying plasmon pole (and, also, the interband edge). The broadening, combined with the low spectral weight, may make the plasmon difficult to observe.

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