Effective-Field Theory of Local-Moment Formation in Disordered Metals

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We present a simple new effective-field theory for the metallic state of a disordered interacting Fermi liquid, taking into account its instability towards the formation of local-moment states. We find a generalization of the compensation theorem of the single-impurity Anderson model, namely, that strongly localized magnetic instabilities occur even when the mean-field single-quasiparticle states are extended. The theory clarifies the understanding of recent thermodynamic and spin-resonance measurements in phosphorus-doped silicon.

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Many theoretical analyses[1,2] have recently addressed the subject of the metal-insulator transition (MIT) in a disordered interacting-electron gas. Using a renormalized weak-disorder perturbation theory, but including the effect of interactions exactly within lowest order in disorder, these investigations have led to an understanding of many transport properties in the disordered metallic phase. However, these theories remain unsatisfactory in explaining the low-temperature thermodynamics as well as the region near the MIT.[3-7] Here we present a new mean-field theory of the *disordered metallic state.* Our theory is directly motivated by experiments on doped semiconductors and should serve as an improved starting point for a complete theory of the MIT.

We take a point of view that is complementary to recent approaches;[2] we treat the noninteracting disordered Hamiltonian *exactly* in a numerical calculation, but account for the interactions in a Hartree-Fock-type approximation.[8] Such an approach is crucial in accounting for the instability of an interacting-electron gas towards the formation of localized magnetic states.[9] This instability is not directly apparent in a disorder perturbation theory even though it can occur for *weak* disorder. Additional motivation comes from the understanding of the insulator through magnetic and optical measurements in doped semiconductors[10] where a correct treatment of disorder effects was crucial.

We discuss our approach in the framework of a disordered Anderson-Hubbard model,

$$H=-\sum_{i\neq j,\,\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i}Un_{i\uparrow}n_{i\downarrow}+\sum_{i,\sigma}(\epsilon_i-\mu)c_{i\sigma}^{\dagger}c_{i\sigma}\,,$$

where i,j extend over all the sites in the system (not necessarily on a lattice), $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$, and σ is the spin index. The off-diagonal disorder in the hopping matrix elements t_{ij} will produce local environments favoring the formation of local moments; we present below a theoretical criterion for this to occur. The on-site energies ϵ_i are weakly random variables $[\langle(\epsilon_i-\langle\epsilon_i\rangle)^2\rangle<\max(t_{ij})]$. We find that an appreciable number of local moments can occur in weak disorder under conditions in which the mean-field single-quasiparticle states near the Fermi level are extended. The localization length of the local moments appears to be finite even in the metallic state; this strong localization may be viewed as a *generalization of the compensation theorem*[9] *for the single-impurity Anderson model.*

We begin by reviewing a well understood special case of H; the *single*-impurity[9] Hamiltonian H_S. We obtain H_S by placing sites i,j on a cubic lattice with hopping matrix elements $t_{ij}=t$ for all nearest-neighbor bonds except for the six bonds connected to the impurity site 0, for which $t_{0i}=t_{i0}=w$. We choose a density of one electron per site ($\epsilon_i=0$, $\mu=U/2$). For $w=0$, a single electron at the origin has energy $-U/2$, while a second electron will cost energy $U/2$; for small w, therefore, the model is related by a canonical transformation to the *symmetric* Anderson model. Using the extensive numerical and analytic renormalization-group analyses[11] on this model, the temperature dependence of the local spin susceptibility of the site 0, χ_0, can be obtained (Fig. 1). At high temperatures, $T\gg U$, interactions are irrelevant and $\chi_0=(g\mu_B)^2/8kT$. For $T<U$ two types of behavior occur. (i) For small w, χ_0 is enhanced to $(g\mu_B)^2/4kT$ at intermediate temperatures due to the formation of a local moment at the origin, but is eventually quenched by the Kondo effect at $T\ll T_K$ (the Kondo temperature). (ii) For larger w one obtains a Fermi liquid[12] and the susceptibility is directly quenched via the onset of the Pauli spin susceptibility. The boundary between these two types of behavior sketched in Fig. 1 is obtained as described below.

Some features of the local-moment formation deserve mention. (i) The Hartree-Fock calculation is adequate to determine the boundary between the local-moment and Fermi-liquid regimes.[11] The Kondo effect, which needs renormalization-group methods, only becomes important at $T\leq T_K$. (ii) In the Fermi-liquid regime, we may perform a nonmagnetic Hartree-Fock factorization of H_S to obtain $(H_S)_{\rm HF}=\sum t_{ij}c_{i\sigma}^{\dagger}c_{i\sigma}$. $(H_S)_{\rm HF}$ is a single-impurity Hamiltonian which can be exactly diagonalized

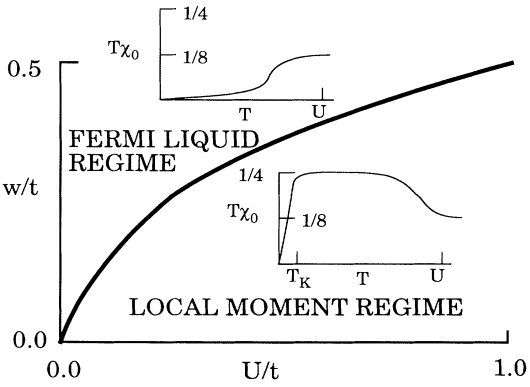

FIG. 1. Phase diagram of the single-impurity Hubbard Hamiltonian H_S; all the nearest-neighbor hopping matrix elements are t except those of the impurity site, which are w. The dark line, representing the *crossover* between the Fermi-liquid and local-moment regimes is determined by an effective-field calculation at $T=0.1w$ for a $6\times6\times6$ cube with periodic boundary conditions (the finite temperature rounds out the divergence in the susceptibility arising from particle-hole symmetry; this divergence is clearly special to H_S). The two regimes are characterized by an impurity spin susceptibility χ_0 of the forms shown in the insets.

by elementary methods; all eigenstates are *extended* with the impurity merely providing a scattering phase shift. The electron local-moment state is associated with a resonance peak *at the Fermi level* in the local density of states at the origin.[9] (iii) The temperature range $T_K \ll T \ll U$ can be quite large for a single impurity. Estimates for T_K in doped semiconductors indicate that it is well below the temperature range that has so far been accessed in experiments. Moreover, it has recently been argued that in a disordered system the effective Kondo temperature T_K is zero.[6]

We now apply the above ideas to the disordered metal described by the fully random H. Assuming that the process of local-moment formation is similar to that in H_S, we see that in the temperature range $T_K < T < U$ the physical properties can be understood by a mean-field treatment of interactions while treating disorder exactly. We use a variant of the effective-field method[13] by finding the single-particle Hamiltonian $H_{\rm eff}$ which best approximates the properties of the interacting system (the response functions obtained from such an approach are guaranteed to satisfy all the conservation laws of the system[13]):

$$H_{\rm eff}(\tilde{\epsilon}_i,\mathbf{h}_i) = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i,\sigma} (\tilde{\epsilon}_i - \mu) c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_i \mathbf{h}_i \cdot \mathbf{S}_i ,$$

where $S_i^{\nu} = c_{i\alpha}^{\dagger} \sigma_{\alpha\beta}^{\nu} c_{i\beta}/2$ is the spin of the electron at site i (σ^{ν} are the Pauli matrices). The Hamiltonian $H_{\rm eff}$ is a function of the variational parameters $\tilde{\epsilon}_i$ and $\mathbf{h}_i$ representing the local site energy and the local magnetic field, respectively. The true free energy F is bounded above by $F_{\rm eff} = \langle H \rangle_{\rm eff} - TS_{\rm eff}$, where $\langle H \rangle_{\rm eff}$ is the expectation value of H in the canonical ensemble defined by $H_{\rm eff}$ and $S_{\rm eff}$ is the entropy of $H_{\rm eff}$ at a temperature T.[13] Consequently, the best variational wave function built up as a Fermi sea of quasiparticles is given by minimizing $F_{\rm eff}$ with respect to $\tilde{\epsilon}_i$ and $\mathbf{h}_i$. As $\mathbf{h}_i = 0$ at high T, we expand to lowest order in the $\mathbf{h}_i$. Let λ_α be the eigenvalues and $\Psi_\alpha(i)$ be the corresponding wave functions of $H_{\rm eff}$ with $\mathbf{h}_i = 0$. Then the condition that $F_{\rm eff}(\tilde{\epsilon}_i, \mathbf{h}_i = 0)$ be a local minimum with respect to $\tilde{\epsilon}_i$ yields the self-consistency equation

$$\tilde{\epsilon}_i = \epsilon_i + U \sum_\alpha |\Psi_\alpha(i)|^2 f(\lambda_\alpha) , \qquad (1)$$

where f is the Fermi function. This equation can be solved to determine the values of $\tilde{\epsilon}_i$. Expanding to second order in the $\mathbf{h}_i$, we obtain

$$F_{\rm eff}(\tilde{\epsilon}_i,\mathbf{h}_i) = F_{\rm eff}(\tilde{\epsilon}_i,\mathbf{h}_i=0) + \sum_{i,j,k} \frac{\chi_{ij}}{4} (\delta_{jk} - U\chi_{jk})(\mathbf{h}_i \cdot \mathbf{h}_k) + \mathcal{O}(\mathbf{h}_i^4) ,$$

where

$$\chi_{ij} = -\sum_{\alpha,\beta} \Psi_\alpha(i) \Psi_\beta^*(i) \Psi_\alpha^*(j) \Psi_\beta(j) \frac{f(\lambda_\alpha) - f(\lambda_\beta)}{\lambda_\alpha - \lambda_\beta} \qquad (2)$$

is the spin susceptibility of free electrons described by $H_{\rm eff}$. Let us denote the eigenvalues of the matrix χ_{ij} by $m_\alpha(i)$ and the corresponding eigenvalues by κ_α [i.e., $\sum_j \chi_{ij} m_\alpha(j) = \kappa_\alpha m_\alpha(i)$]. It is clear from Eq. (2) that $\mathbf{h}_i$ will first become nonzero when $\max(\kappa_\alpha)$ becomes larger than $1/U$. The distribution of the magnetization corresponding to this instability will be given by the eigenvector $m_\alpha(i)$ associated with the largest eigenvalue.

For the single-impurity Hamiltonian H_S at half-filling, particle-hole symmetry gives the constraint $\mu = \tilde{\epsilon}_i = U/2$; the self-consistency equation (1) is therefore trivially solvable. We found numerically that the eigenvalues of χ_{ij} form a continuous band with a single eigenvalue, κ_β, split off from the top of the band; thus $\kappa_\beta = 1/U$ determines the boundary line in Fig. 1 for the formation of a local moment. For small w, the eigenvector $m_\beta(i)$ associated with the largest eigenvalue κ_β is *localized* around the origin. This occurs even though all of the eigenstates of $H_{\rm eff}$, $\Psi_\alpha(i)$, are *extended*. The localization of $m_\beta(i)$ is closely linked to the compensation theorem of Anderson[9] which is valid in the limit of infinite bandwidth.

Returning to the disordered Hamiltonian H, we focus on a particular realization of the disorder, motivated by the doped semiconductors such as phosphorus-doped silicon (Si:P). It consists of sites placed *randomly* in space at positions $\mathbf{r}_i$; t_{ij} are given by the Heitler-London approximation for $1s$ hydrogenic wave functions[14] $|t_{ij}| = 2t_0(1 + |\mathbf{r}_{ij}|/a)e^{-|\mathbf{r}_{ij}|/a}$, where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, a is the Bohr radius, and $t_0 = 1$ Ry. Using the binding energies of the H atom and the H^- ion we get $U = 0.95$ Ry; consequently, we use $U/t_0 = 1$ in our calculations. Choosing a larger (smaller) value of U/t increases (decreases) the number of local moments obtained at a given density but does not affect our conclusions qualitatively. We as-

sumed that ϵ_i was distributed uniformly between $-t_0/10$ and $t_0/10$ (the results were quite insensitive to the presence of this diagonal disorder as long as the width of the distribution of the ϵ_i was not of order t_0). In Si:P, the donor electrons are bound to phosphorus nuclei in $1s$-like states derived from many conduction-band minima. Interference between various silicon band wave functions leads to a random sign in the hopping matrix element,[15] a feature which we include by assigning a random sign to each t_{ij}. The MIT for this Hamiltonian is expected to occur near the canonical Mott value $\rho=\rho_c$ given by $\rho_c a^3 \approx 0.016$.[14,16] We therefore performed our calculations at densities around this value with electron filling factors between 0.4 and 1 electron per site for sizes between 50 and 300 sites placed randomly in a cubic box. The system was periodically continued in all directions, and the t_{ij} were computed using the *shortest* distance between every pair of sites. We averaged between 5 and 20 samples for each size, density, and filling factor.

The first step was solving the self-consistency equation (1) iteratively for the renormalized local site energies. For a density of 1 electron site, we find $\mu \approx \tilde{\epsilon}_i \approx U/2$ indicating the presence of an average particle-hole symmetry (the particle-hole symmetry is not exact because of the presence of loops with an add number of sites). The next step was the evaluation of the matrix χ_{ij} using Eq. (2) and its diagonalization (the computer time required to initialize the matrix χ_{ij} limited the size of the system we could simulate). We determined the eigenvalues κ_α and the corresponding eigenvectors $m_\alpha(i)$ of χ_{ij}. All eigenvalues of χ_{ij} satisfying $\kappa_\alpha > 1/U$ represent potential local-moment instabilities. To ensure that these represented *independent* local moments [i.e., the eigenvectors $m_\alpha(i)$ were localized and well separated from each other], we evaluated the cross inverse participation ratio

$$P_{\alpha\beta}=\frac{\sum_i |m_\alpha(i)|^2 |m_\beta(i)|^2}{[\sum_i |m_\alpha(i)|^4]^{1/2}[\sum_i |m_\beta(i)|^4]^{1/2}}.$$

Only the larger of a pair of eigenvalues κ_α and κ_β with $P_{\alpha\beta} > P_m$ was accepted as representing a local moment. We chose values of P_m between 0.1 and 0.5. Variations of P_m in this range produced relative changes in the number of local moments which varied from $<1\%$ at high temperatures and high densities up to $\sim 25\%$ at the lowest temperatures and densities.

We first discuss the case of a density of 1 electron per site (this corresponds to uncompensated Si:P). The calculations were carried out at temperatures of $T=0.1t_0$ and $T=0.01t_0$ for a number of sample sizes and densities. We found that, at a fixed density of electrons, the number of local moments was quite accurately proportional to the total number of electrons for system sizes greater than twenty sites. This is as would be expected if the system size is much greater than the localization length of the local moments. The ratio of the number of local-moment instabilities to that of electrons was found to increase monotonically with decreasing density from 1% at $\rho a^3=0.03$ to 16% at 0.01. We show below that the (spin) localization length associated with the local moments is not directly related to the (charge) localization length of the electrons, and is much smaller than it.

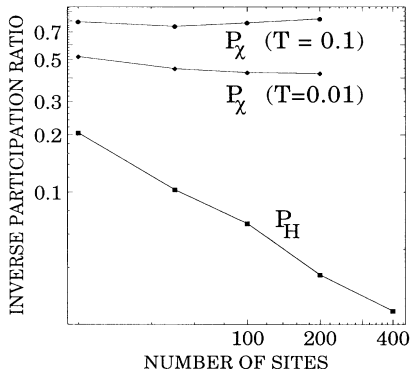

FIG. 2. Mean inverse participation ratio P_H of the eigenvectors $\Psi_\alpha(i)$ of H, and P_χ of the eigenvectors $m_\alpha(i)$ of χ, at a density $\rho a^3=0.02$, and the filling factor $\approx \frac{1}{2}$ for different sizes. We used an upper cutoff $P_m=0.5$ for the cross inverse participation ratio $P_{\alpha\beta}$. The values of P_χ are shown at two temperatures (measured in units of t_0); they are *independent* of system size suggesting that the eigenvectors $m_\alpha(i)$ are localized. Values of P_H show no appreciable T dependence and decrease with system size suggesting that the $\Psi_\alpha(i)$ are extended.

We also studied the properties of the single-particle wave functions, $\Psi_\alpha(i)$, and the eigenvectors, $m_\alpha(i)$, of χ_{ij}. Although there is no simple relationship between these two sets of eigenvectors, our experience shows that every eigenvector $m_\alpha(i)$ which is localized around the site $\mathbf{r}_k$ (say) is associated with an eigenvector $\Psi_\alpha(i)$ which is peaked at $\mathbf{r}_k$ and has an eigenenergy *close to the Fermi level*. Exactly the same correspondence is present in the single-impurity Hamiltonian H_S. We evaluated the inverse participation ratios $P_{H\alpha}=\sum_i |\Psi_\alpha(i)|^4$ and $P_{\chi\alpha}=\sum_i |m_\alpha(i)|^4$. We plot in Fig. 2 the average of $P_{H\alpha}$, $P_H=\langle P_{H\alpha}\rangle$ over many samples and for states within $0.1t_0$ of the Fermi energy for a fixed density of electrons $\rho a^3=0.02$. On a log-log plot, P_H decreases monotonically as a function of the number of sites in the system with a slope $\simeq 0.73$, which is reasonable since the correlation length is comparable to system size, and is evidence that all the states within $0.1t_0$ of the Fermi level are *extended*. For the same samples, the behavior of $P_\chi=\langle P_{\chi\alpha}\rangle$ is quite different. It remains *independent* of the system size at a value of around 0.5 (for $T=0.01t_0$) showing quite convincingly that all of the local-moment states are *localized* on length scales of order the spacing between the sites (at higher temperatures P_χ increases towards its $T=\infty$ limit of $P_\chi=1$).

All of the above discussion has concentrated on an electron filling factor of 1 electron per site. As in the single-impurity Anderson model, this is the most favorable condition for the formation of local moments. To explore the consequences of changing the number of

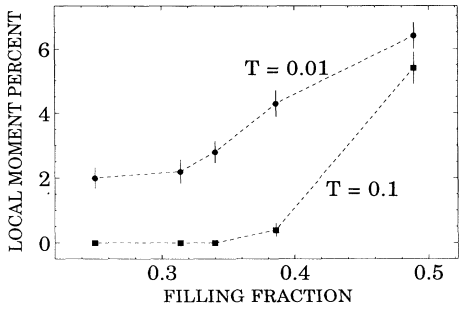

FIG. 3. The ratio of the number of local moments to the total number of electrons, $f_{\rm lm}$, as a function of filling factor for a constant density of electrons $\rho a^3=0.02$ at two different temperatures (measured in units of t_0).

electrons per site we repeated all of the calculations with decreasing values of the chemical potential μ down to a filling fraction of 0.25. We show in Fig. 3 results for $f_{\rm lm}$, the ratio of the number of local-moment instabilities to the total number of *electrons*, as a function of filling factor for a constant density of electrons $\rho a^3=0.02$. The value of $f_{\rm lm}$ in an effective-field calculation increases with falling temperature; at $T=0.01t_0$, $f_{\rm lm}$ is expected to be close to its asymptotic zero-temperature value. We see from Fig. 3 that $f_{\rm lm}$ is a maximum at half-filling; however, the falloff with decreasing filling fraction is rather gradual.

While our calculations have been done on a model Hamiltonian, we have chosen the model to capture the essential aspects of disorder and electron correlation. It is thus gratifying that our estimate for the number of local-moment instabilities of $\sim 10\%$ of the sites at densities within 50% of the critical density ρ_c is in good agreement with experimental estimates of 10%–25% from NMR [3] and thermodynamic [5] measurements. A larger U/t_0 suggested by Ref. 15 would in fact improve agreement. We regard this agreement to be a vindication of the basic physical picture of the phenomenological two-fluid (the itinerant electrons and the localized moments) model of metallic doped semiconductors. [3,5,17]

To conclude, we have shown in this paper that a system of interacting electrons in weak disorder displays a strong instability towards the formation of localized moments on length scales much shorter than the localization length of the electrons' Hartree-Fock wave functions. This phenomenon has been argued to be related to the *compensation theorem* of the single-impurity Anderson model where competing ferromagnetic (due to the spatial extent of the impurity wave function) and antiferromagnetic interactions (due to superexchange) cancel each other, leading to a very localized spin polarization. Any complete theory of the MIT has therefore to account for the presence of the electron local moments and the effect of interactions between the local moments and the itinerant electrons. Two steps in this direction have been taken: (a) the determination of the Fermi-liquid properties of a two-fluid model of itinerant electrons and local moments [18] and (b) the study of the very low-temperature properties of a disordered system with local moments. [6] An important question which remains open is the precise role of the local-moment instabilities in the critical behavior of charge transport near the MIT.

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