Attractive Interaction and Pairing in Fermion Systems with Strong On-Site Repulsion

J. E. Hirsch
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 19 November 1984)

It is shown that an effective attractive interaction between nearest-neighbor antiparallel spins arises in the Hubbard and Anderson lattice models in the limit of large on-site electron-electron repulsion. Results of Monte Carlo simulations of the Hubbard model show enhancement of anisotropic singlet-pairing correlations and suppression of triplet-pairing correlations. It is proposed that this interaction leads to an anisotropic singlet superconducting state in the heavy-fermion superconductors.

PACS numbers: 75.10.Hk, 74.20.−z

The discovery of superconductivity in heavy-fermion systems[1] has posed many interesting questions, in particular whether it is the first example of non-phonon-induced superconductivity. It has been suggested that these systems exhibit triplet superconductivity,[2,3] with the attractive interaction due to paramagnon exchange.[3] Other theoretical treatments assume the usual BCS state induced by electron-phonon interactions.[4]

Two models of interacting fermions, the Hubbard and Anderson models, have been used to describe these systems.[5-7] While the Anderson model is closer to the real materials, the Hubbard model is simpler and probably shares some of its features. Here, we study these models in the strong-coupling limit. The Hubbard model is defined by

$$H=-t\sum_{\substack{\langle i,j\rangle\\ \sigma}}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}. \tag{1}$$

In the limit of large U, H reduces to an antiferromagnetic Heisenberg (AFH) model in the half-filled band case (one electron per site).[8] Klein and Seitz[9] showed that an AFH model still describes the *spin* degrees of freedom for other than half-filled cases in one dimension in strong coupling. Here, we derive an effective Hamilonian for the spin *and charge* degrees of freedom. We take as zeroth-order Hamiltonian the interaction term, and as perturbation the hopping. The ground state to zeroth order is highly degenerate, consisting of an arbitrary arrangement of *singly occupied* sites. To first order, the kinetic-energy term forms a band described by the Hamiltonian

$$H_1=-t\sum_{\substack{\langle i,j\rangle\\ \sigma}}(h_{i\sigma}^{\dagger}h_{j\sigma}+\text{H.c.}). \tag{2}$$

The operators $h_{i\sigma}$ hop single electrons from site to site but are not true fermion operators since they do not allow double occupancy, i.e., $h_{i\uparrow}^{\dagger}h_{i\downarrow}^{\dagger}=0$. In one dimension, it is easy to see that Eq. (2) describes a noninteracting gas of *spinless fermions*. In higher dimensions the properties of the Hamiltonian of Eq. (2) are unknown, but it is plausible to assume that the system can be described by a Fermi liquid of spinless fermions as far as the charge degrees of freedom are concerned, by analogy with one dimension. Such a system should become unstable in the presence of a small attractive interaction.

To next order in t/U, we allow for virtual transitions into states with doubly occupied sits. The effective Hamiltonian, acting only on the states with single occupied sites, is

$$H_{\text{eff}}=-t'\sum_{\substack{\langle i,j\rangle\\ \sigma}}(h_{i\sigma}^{\dagger}h_{j\sigma}+\text{H.c.})-V'\sum_{\langle i,j\rangle}n_in_j+V'\sum_{\langle i,j\rangle}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j+\frac{V'}{2}\sum_{\substack{\langle i_1,i_2,i_3\rangle\\ \sigma}}(h_{i_1,\sigma}^{\dagger}n_{i_2,-\sigma}h_{i_3,\sigma}+\text{H.c.})$$
$$-\frac{V'}{2}\sum_{\substack{\langle i_1,i_2,i_3\rangle\\ \sigma}}(h_{i_1,\sigma}^{\dagger}h_{i_2,-\sigma}^{\dagger}h_{i_2,-\sigma}h_{i_2,\sigma}h_{i_3,-\sigma}+\text{H.c.}), \tag{3}$$

where i_1, i_2, and i_3 are neighboring sites, $n_{i\sigma}=h_{i\sigma}^{\dagger}h_{i\sigma}$, $n_i=n_{i\uparrow}+n_{i\downarrow}$, $t'=t$, and $V'=2t^2/U$. Note that an effective attraction between nearest-neighbor electrons occurs, as a reuslt of virtual transitions to the excluded doubly occupied states. Actually, the attraction is only between antiparallel spins; the one between parallel spins is canceled by the third term in the Hamiltonian, a nearest-neighbor antiferromagnetic exchange. The last two terms in H describe the hopping of pairs of nearest-neighbor electrons with opposite spin, with and without spin flip.

Figure 1 shows the nearest-neighbor charge-density correlation function $\langle n_in_{i+1}\rangle$ in the ground state of a four-site Hubbard chain with two electrons of opposite spin. Note that it *increases* as U decreases, because of the nearest-neighbor attraction discussed above, and peaks around $U\sim 4$ (in units of t). The results obtained from the effective Hamiltonian of Eq. (3) are shown as the dotted line. Exact diagonalizations up to

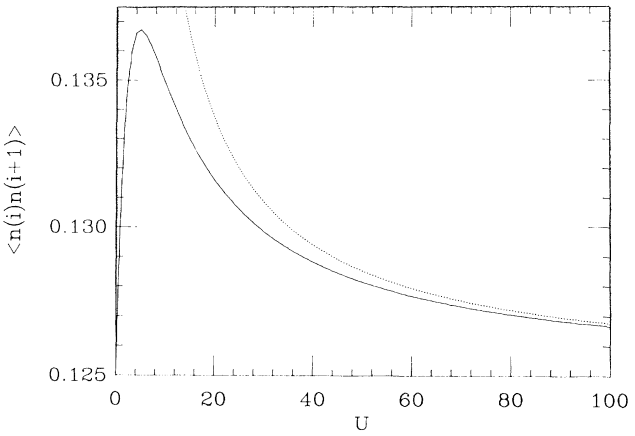

FIG. 1. Nearest-neighbor charge-density correlations in a four-site Hubbard model with two electrons of opposite spin. The dotted line shows the results obtained from the effective Hamiltonian, Eq. (3).

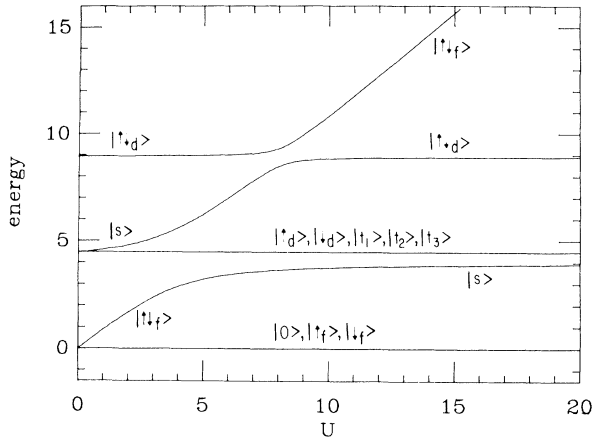

FIG. 2. Lowest-energy level vs U for a single-site Anderson model with $\epsilon_d-\epsilon_f=4$, $V=1$. The subindex (d or f) in a state indicates that the state is predominantly of that character, with a small admixture of states of the other band. s and t refer to singlet and triplet states. ϵ_f is chosen so that the states $|0\rangle$, $|\uparrow_f\rangle$, and $|\downarrow_f\rangle$ are degenerate.

eight sites and Monte Carlo simulations for systems up to 64 sites in one and two dimensions show that the qualitative behavior shown in Fig. 1 always occurs for band fillings not too far from $\frac{1}{4}$.[10]

For systems where the intersite hopping occurs through direct overlap of the atomic wave functions, like transition metals, we do not expect this effective attractive interaction to play a role, since it will be overwhelmed by the larger nearest-neighbor direct Coulomb repulsion. However, as is shown below, we obtain the same effective Hamiltonian to describe the f electrons in the Anderson model. For the heavy-fermion superconductors, there is probably no direct f-f overlap[1] so that this cancellation would not occur.

We consider the Anderson lattice Hamiltonian

$$H=-t\sum_{\substack{\langle i,j\rangle\\ \sigma}}(d_{i\sigma}^{\dagger}d_{j\sigma}+\text{H.c.})+V\sum_{i}(d_{i\sigma}^{\dagger}f_{i\sigma}+\text{H.c.})+\epsilon_d\sum_{i,\sigma}n_{di,\sigma}+\epsilon_f\sum_{i,\sigma}n_{fi,\sigma}+U\sum_{i}n_{fi\uparrow}n_{ni\downarrow}, \tag{4}$$

and start by solving the site problem, i.e., $t=0$. The lowest-energy levels as a function of U are shown in Fig. 2 for a particular case. We will keep only the states labled $|0\rangle$, $|\uparrow_f\rangle$, and $|\downarrow_f\rangle$. These states are essentially f-electron states, with a small admixture [of order $V/(\epsilon_d-\epsilon_f)$] of d-electron states. We take into account the influence of the higher states in perturbation theory in t,[11] and keep only the dominant contributions to second order, involving transitions to the states labeled $|\uparrow_d\rangle$, $|\downarrow_d\rangle$, $|t_1\rangle$, $|t_2\rangle$, $|t_3\rangle$, and $|s\rangle$ in Fig. 2 (this effectively amounts to our taking $U=\infty$). Details of the calculation will be given elsewhere. The result is an effective Hamiltonian identical to Eq. (3) for the "renormalized" f electrons, with

$$t'=[V^2/(\epsilon_d-\epsilon_f)^2]t, \tag{5a}$$

$$V'=2V^4t^2/(\epsilon_d-\epsilon_f)^5, \tag{5b}$$

to lowest order in $V/(\epsilon_d-\epsilon_f)$ (the general expressions will be given elsewhere). Here, the effective attraction has a different origin than in the Hubbard case: It arises from the fact that the energy of the singlet state for $U\rightarrow\infty$ is lowered from its energy at $U=0$ (see Fig. 2) by the Kondo coupling

$$\Delta E=4J_{\text{eff}}=2V^2/(\epsilon_d-\epsilon_f), \tag{6}$$

to lowest order in $V/(\epsilon_d-\epsilon_f)$, as one would expect from the Schrieffer-Wolff transformation.[12] A similar expansion for $U=0$ gives attractive and repulsive interactions that exactly cancel because of the degeneracy of the singlet and triplet states.

As mentioned earlier, we do not expect a direct nearest-neighbor repulsion between f electrons in the heavy-fermion systems because of the large separation between f atoms.[1] Still, a nearest-neighbor repulsion V_c between the d electrons in the Hamiltonian of Eq. (4) would contribute an effective repulsion between the renormalized f electrons. Because of screening by the conduction electrons V_c is likely to be quite small, so that its contribution to the effective interaction, which is further reduced by f-d overlap matrix elements, is probably negligible. A detailed quantitative estimate, however, has not been performed.

Our effective Hamiltonian for the Anderson model describes "heavy" f electrons, since the effective hop-

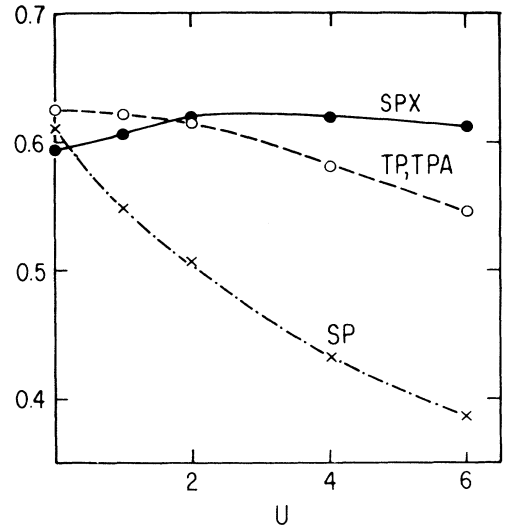

FIG. 3. Pairing-correlation functions at $q=0$ vs U for a 6×6 Hubbard model at $\beta=3$, band filling $\rho=0.67$, from Monte Carlo simulations. The statistical error is smaller than the points.

ing t' [Eq. (5a)] is probably quite small in these systems. Because of the effective attraction, one might expect pairing correlations to develop at low temperatures. One potential use of this effective Hamiltonian is for exact diagonalization studies: Since the Hilbert space has only two states per site, much larger systems can be studied than for the full Anderson or Hubbard models. Here, we use the effective Hamiltonian only as a guide, which suggests that one might have a tendency towards pairing of electrons on neighboring sites and antiferromagnetism. We have studied static correlation functions of the form

$$S_0(q)=N^{-1}\sum\exp[iq(R_i-R_j)]\langle O_iO_j^{\dagger}\rangle \qquad (7)$$

in the Hubbard model by Monte Carlo simulations,[13] with O_i pairing operators of the form

$$\begin{aligned} O_i&=c_{i\uparrow}c_{i\downarrow} \quad \text{(SP)},\\ O_i&=c_{i\uparrow}c_{i+\hat{x}\downarrow}-c_{i\downarrow}c_{i+\hat{x}\uparrow} \quad \text{(SPX)},\\ O_i&=c_{i\uparrow}c_{i+\hat{x}\uparrow} \quad \text{(TP)},\\ O_i&=c_{i\uparrow}c_{i+\hat{x}\downarrow}+c_{i\downarrow}c_{i+\hat{x}\uparrow} \quad \text{(TPA)}, \end{aligned} \qquad (8)$$

for singlet pairing (SP), extended singlet pairing (SPX), and triplet pairing of parallel (TP) and of antiparallel (TPA) spins. Figure 3 shows the dependence on U on a 6×6 two-dimensional lattice at temperature $\beta=3$ and band filling $\rho=0.67$. Qualitatively similar results were obtained for a three-dimensional $4\times4\times4$ lattice. It can be seen that $S_{\rm SPX}(q=0)$ is enhanced by the Hubbard interaction, while the others are suppressed (the results for $S_{\rm TP}$ and $S_{\rm TPA}$ are identical within statistical error). Since we derived the same effective Hamiltonian in strong coupling for the Anderson and Hubbard models, we expect these results for the Hubbard model to be relevant to the Anderson model in the appropriate regime. For other band fillings, the results are qualitatively similar to Fig. 3, with the effect of U becoming smaller as the band filling decreases. In particular, we never found enhancement of triplet-pairing correlations.

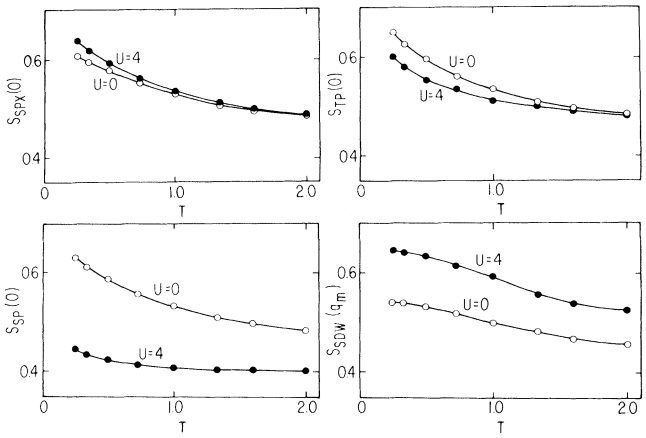

FIG. 4. Temperature dependence of pairing and spin-density-wave (SPW) correlations for a 6×6 Hubbard model, $\rho=0.67$.

Figure 4 shows the temperature dependence of the pairing correlations and of the spin-density correlations for $U=4$, $\rho=0.67$. The q value for which $S_{\rm SDW}$ is maximum, q_m, is close to (π,π) and somewhat temperature dependent. $S_{\rm SDW}$ is strongly enhanced, but the ratio to the $U=0$ values is approximately constant as T decreases. $S_{\rm SPX}$ instead is further enhanced as T is lowered. If $S_{\rm SPX}(q=0)$ were to diverge at a critical temperature, it would signal a transition to a singlet superconducting state with an anisotropic energy gap of the form

$$\Delta(k)=\Delta(\cos k_x+\cos k_y+\cos k_z) \qquad (9)$$

in a simple cubic lattice. Such a state was discussed by Ohkawa and Fukuyama.[14] Because the gap can vanish along a line on the Fermi surface, the system can exhibit power-law temperature dependence of the specific heat and ultrasonic attenuation instead of the usual exponential dependence, as is found in UBe_{13} and UPt_3.[1]

In summary, we have shown that an effective nearest-neighbor attraction arises in fermion systems with strong on-site repulsion. This attractive interaction leads to enhancement of extended singlet-pairing correlations, as demonstrated by our Monte Carlo simulation results on the Hubbard model. We derived an effective Hamiltonian for the Anderson model which describes a narrow band of heavy electrons with an interaction that can lead to an anisotropic singlet su-

perconducting state at low temperatures with features analogous to those found in the heavy fermion systems, induced solely by the strong on-site electron-electron repulsion.

The computations reported here were performed on the Cray-1 computer at the University of Minnesota, funded through the National Science Foundation program for access to supercomputers. In addition, this work was supported by the National Science Foundation under Grant No. DMR-82-17881 and by the Alfred P. Sloan Foundation through a research fellowship.

[1]G. R. Stewart, Rev. Mod. Phys. **56**, 755 (1984), and references therein.

[2]C. M. Varma, to be published.

[3]P. W. Anderson, Phys. Rev. B **30**, 1549 (1984).

[4]H. Razafimandimky, P. Fulde, and J. Keller, Z. Phys. **54**, 111 (1984).

[5]M. Taichiki and S. Maekawa, Phys. Rev. B **29**, 2497 (1984).

[6]N. Grewe, Z. Phys B **56**, 111 (1984).

[7]K. Ueda and T. M. Rice, to be published.

[8]V. J. Emery, Phys. Rev. B **14**, 2989 (1976).

[9]D. J. Klein and W. A. Seitz, Phys. Rev. B **10**, 3217 (1974).

[10]J. E. Hirsch, unpublished.

[11]We have recently studied a Kondo lattice model in perturbation theory in t (J. E. Hirsch, to be published), for a different regime, however, than the one considered here.

[12]J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).

[13]J. E. Hirsch, Phys. Rev. Lett. **51**, 1900 (1983); J. E. Hirsch and D. J. Scalapino, Phys. Rev. Lett. **53**, 706 (1984).

[14]F. Ohkawa and H. Fukuyama, to be published.