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Effective electron-electron interaction in the two-dimensional Hubbard model

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The structure of the effective electron-electron interaction in the doped two-dimensional Hubbard model is examined. Monte Carlo results for the irreducible electron-electron vertex in the singlet channel are compared with a spin-fluctuation exchange approximation for the effective interaction. We conclude that the exchange of paramagnetic-antiferromagnetic spin fluctuations mediates the effective-pairing interaction in the weak-to-moderately-coupled Hubbard model.

One approach to describing the mechanism for high-temperature superconductivity focuses on the characteristic fluctuations in a given model and the nature of the effective interaction which the exchange of these fluctuations mediates. For example, the dominant fluctuations in the doped Hubbard model are paramagnetic-antiferromagnetic spin fluctuations and it has been suggested that the effective electron-electron interaction in the weak-to-moderately-coupled Hubbard model is mediated by the exchange of these fluctuations.[1,2] However, the degree to which such a fluctuation exchange interaction provides an accurate representation is not known. In particular, do single spin-fluctuation exchange processes dominate or are higher-order multiple-spin-fluctuation[3,4] exchanges essential? What about vertex corrections?[5–7] Here we examine these questions for the Hubbard model by comparing quantum Monte Carlo results for the irreducible vertex with an effective interaction describing the single exchange of a spin fluctuation. Our goal is to determine the extent to which the Monte Carlo results for the irreducible vertex can be adequately modeled by a single spin-fluctuation exchange. We will also examine the spatial structure of the interaction to obtain additional physical insight into its nature. Previously, we studied the eigenvalues and eigenfunctions of the Bethe-Salpeter equation associated with this vertex.[8,9] Here we focus directly on the structure of the interaction and its relationship to the underlying antiferromagnetic spin fluctuations.

The calculations which will be discussed were carried out for a two-dimensional Hubbard model with the Hamiltonian

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

Here $c_{i\sigma}^{\dagger}$ creates an electron of spin σ on site i,t is a one-electron near-neighbor transfer, and U is the on-site Coulomb interaction. Quantum Monte Carlo simulations[8] were carried out for an 8×8 periodic lattice with $U=4t$ at a filling $\langle n_{i\uparrow}+n_{i\downarrow}\rangle=0.87$. The lowest temperature considered here is $T=t/4$ corresponding to an energy $\frac{1}{32}$ of the bandwidth. If the exchange interaction J were approximated by $4t^2/U$, then for $U=4t$ this temperature would correspond to $J/4$. These calculations provide a description of the interaction on space and time scales which are larger than the characteristic spin-fluctuation correlation length and the inverse of the exchange coupling energy. Thus, while one is significantly above the temperature at which the interaction may induce pairing correlations, the interaction should be well enough formed to obtain useful insight into its basic structure.

The spin fluctuations can be characterized by the magnetic spin susceptibility

$$\chi(\mathbf{q},i\omega_m)=\frac{1}{N}\sum_{l}\int_0^{\beta}d\tau\, e^{i(\omega_m\tau-\mathbf{q}\cdot l)}\langle m_{i+l}^{-}(\tau)m_i^{+}(0)\rangle\ , \tag{2}$$

with $m_i^{-}=c_{i\downarrow}^{\dagger}c_{i\uparrow}$. Here $\omega_m=2m\pi T$ is the usual boson Matsubara frequency and

$$m_i^{-}(\tau)=\exp[(H-\mu N)\tau]m_i^{-}\exp[-(H-\mu N)\tau] \tag{3}$$

with μ the chemical potential. Figure 1(a) shows Monte Carlo results for $\chi(\mathbf{q},0)$ for various temperatures. As T decreases below the characteristic exchange energy, strong antiferromagnetic correlations are seen to develop. In Fig. 1(b), the ω_m dependence of $\chi(\mathbf{q},i\omega_m)$ is shown for $\mathbf{q}=(\pi,\pi)$. The rapid falloff is associated with the spin-fluctuation energy scale.

In the same simulation, the two-particle Green's function G_2 was calculated,

$$G_2(x_4,x_3,x_2,x_1)=-\langle Tc_{\uparrow}(x_4)c_{\downarrow}(x_3)c_{\downarrow}^{\dagger}(x_2)c_{\uparrow}^{\dagger}(x_1)\rangle\ . \tag{4}$$

Here $c_{\sigma}^{\dagger}(x_i)$ with $x_i=(l_i,\tau_i)$ creates an electron of spin σ at site l_i and imaginary time τ_i. T is the usual τ-ordering operator. After taking the Fourier transform of both the

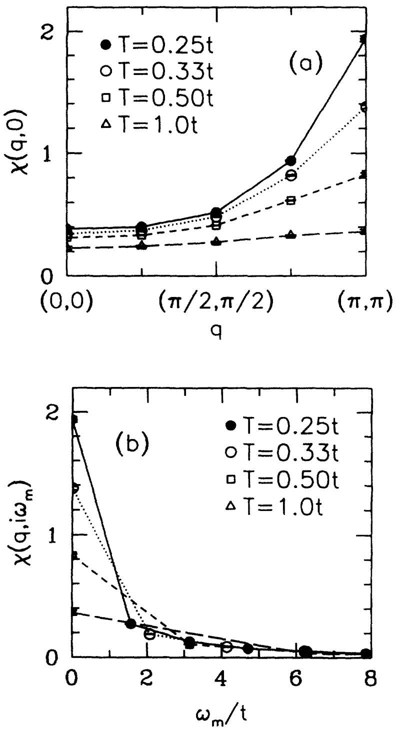

FIG. 1. Momentum dependence of $\chi(\mathbf{q},i\omega_m=0)$ along the (1,1) direction. (b) Matsubara frequency dependence of $\chi(\mathbf{q},i\omega_m)$ for $\mathbf{q}=(\pi,\pi)$. Here results are shown for various temperatures, and χ is given in units where $t=1$.

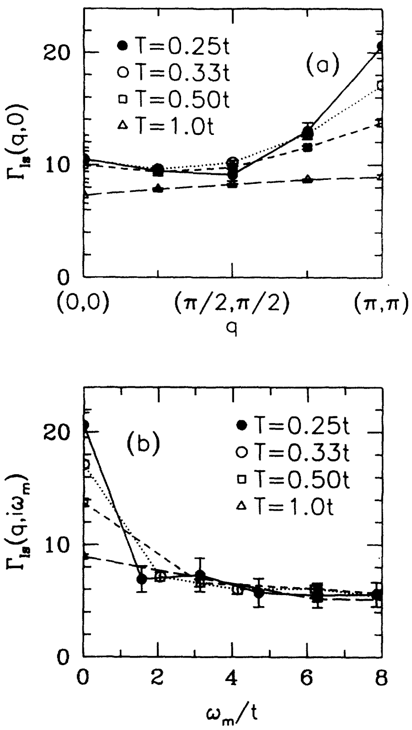

FIG. 2. (a) Momentum dependence of the irreducible vertex in the singlet channel, $\Gamma_{\rm Is}(\mathbf{q},i\omega_m)$, for zero energy transfer $\omega_m=0$. Here the incoming momentum $\mathbf{p}=(\pi,0)$, the outgoing momentum $\mathbf{p}'=\mathbf{p}+\mathbf{q}$, and $\omega_n=\omega_{n'}=\pi T$. (b) Energy-transfer dependence of $\Gamma_{\rm Is}(\mathbf{q},i\omega_m)$ for $\mathbf{q}=(\pi,\pi)$, $\omega_n=\pi T$, and $\omega_{n'}=\omega_n+\omega_m$. Here results are shown for various temperatures, and $\Gamma_{\rm Is}$ is given in units of t.

space and imaginary time variables, G_2 can be expressed in terms of the single-particle Green's function $G_\sigma(\mathbf{p},i\omega_n)$ and the reducible particle-particle vertex $\Gamma(p',k',k,p)$,

$$G_2(p',k',k,p)=-\delta_{p,p'}\delta_{k,k'}G_\downarrow(k)G_\uparrow(p)+\frac{T}{N}\delta_{p'+k',p+k}G_\uparrow(p')G_\downarrow(k')\times\Gamma(p',k',k,p)G_\downarrow(k)G_\uparrow(p)\ . \quad (5)$$

Here $p=(\mathbf{p},i\omega_n)$. Using the Monte Carlo results for G_2 and G, one can determine the reducible vertex $\Gamma(p',k',k,p)$ from Eq. (5). We are interested in studying the pairing correlations in the zero center-of-mass momentum and energy channel; hence we set $k=-p$ and $k'=-p'$. Then, from the t-matrix equation

$$\Gamma_I(p'|p)=\Gamma(p'|p)+\frac{T}{N}\sum_k\Gamma(p'|k)G_\downarrow(-k)G_\uparrow(k)\Gamma_I(k|p) \quad (6)$$

one can solve for the irreducible vertex Γ_I. In Eq. (6), $\Gamma(p'|p)$ denotes $\Gamma(p',-p',-p,p)$.

The irreducible two-particle interaction in the singlet channel is given by

$$\Gamma_{\rm Is}(p'|p)=\tfrac{1}{2}[\Gamma_I(p'|p)+\Gamma_I(-p'|p)]\ . \quad (7)$$

This is the effective electron-electron interaction responsible for pairing in the singlet channel. Here we study the singlet channel, since the fastest growing pairing correlations near half filling are in this channel.[8,9] Figure 2(a) shows Monte Carlo results for $\Gamma_{\rm Is}(\mathbf{q},i\omega_m)$ versus $\mathbf{q}=\mathbf{p}'-\mathbf{p}$ with $\omega_m=\omega_{n'}-\omega_n=0$. As the temperature is lowered, $\Gamma_{\rm Is}$ increases at large momentum transfer. Note that the bare interaction would be equal to a constant value of $4t$. We also observe that the effective interaction created by U becomes large, reaching a value greater than twice the bandwidth at $\mathbf{q}=(\pi,\pi)$. The Matsubara frequency dependence of $\Gamma_{\rm Is}$ for $\mathbf{q}=(\pi,\pi)$ is shown in Fig. 2(b) at various temperatures.

We now compare this with the single-spin-fluctuation exchange interaction

$$\Gamma_I^{\rm SF}(\mathbf{p}',i\omega_{n'}|\mathbf{p},i\omega_n)=U+\tfrac{3}{2}g^2U^2\chi(\mathbf{p}'-\mathbf{p},i\omega_{n'}-i\omega_n)\ . \quad (8)$$

This form is motivated by the Berk-Schrieffer interaction,[10] which basically has this form with $g=1$ near the antiferromagnetic instability. The factor of $\frac{3}{2}$ arises from the two transverse and one longitudinal spin fluctuations. In calculating $\Gamma_{\rm Is}^{\rm SF}$ with Eq. (8), we will use Monte Carlo results for $\chi(\mathbf{q},i\omega_m)$ and also set $g=0.8$. The corresponding value of $3.2t$ for the effective coupling gU is consistent with the results of a Monte Carlo calculation of the irreducible particle-hole vertex which we have carried out.[11,12] Formally, Eq. (8) is analogous to the

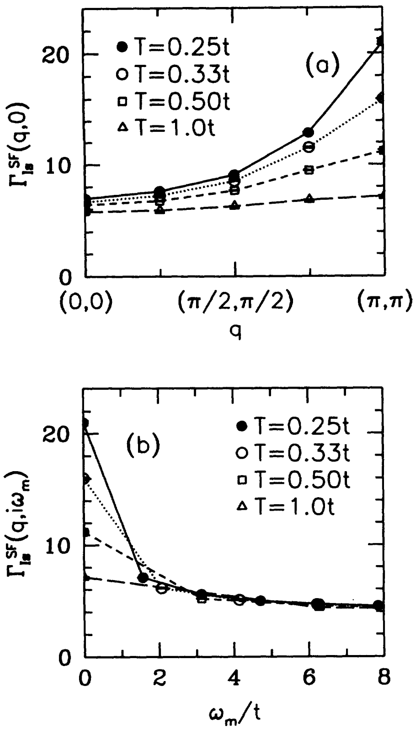

FIG. 3. (a) Momentum and (b) frequency dependence of $\Gamma_{Is}^{SF}(\mathbf{q},i\omega_m)$ obtained from Eq. (8) using $g=0.8$. Here results have been plotted as in Fig. 2.

effective interaction in the electron-phonon superconductor,

$$V(\mathbf{q},i\omega_m)=U+\sum_{\lambda}|g_{\mathbf{q}\lambda}|^2D_\lambda(\mathbf{q},i\omega_m)\ , \tag{9}$$

where $D_\lambda(\mathbf{q},i\omega_m)$ is the dressed phonon propagator and $|g_{\mathbf{q}\lambda}|^2$ is the renormalized electron-phonon coupling.

Figure 3(a) shows $\Gamma_{Is}^{SF}(\mathbf{q},i\omega_m=0)$ versus $\mathbf{q}$ at various temperatures. These results are to be compared with $\Gamma_{Is}(\mathbf{q},0)$ shown in Fig. 2(a). Likewise, Fig. 3(b) shows that the frequency dependence of Γ_{Is}^{SF} is in close agreement with the Monte Carlo results shown in Fig. 2(b). Considering the simplicity of Eq. (8), the agreement with the Monte Carlo data is quite good. These comparisons suggest that a properly renormalized single-spin-fluctuation exchange interaction is capable of reproducing the basic features of the effective particle-particle interaction in the weak-to-intermediate-coupling Hubbard model.

Finally, in order to gain further insight into the structure of the effective particle-particle interaction it is useful to consider the real-space Fourier transform,

+0.01	−0.12	+0.12	−0.12	+0.01
−0.12	+0.43	−0.50	+0.43	−0.12
+0.12	−0.50	+9.6	−0.50	+0.12
−0.12	+0.43	−0.50	+0.43	−0.12
+0.01	−0.12	+0.12	−0.12	+0.01

FIG. 4. Monte Carlo data on the real-space structure of $\Gamma_{Is}(\mathbf{R})$ as defined by Eq. (10). The estimated error in these data is of order 10%.

$$\Gamma_{Is}(\mathbf{R})=\frac{1}{N^2}\sum_{\mathbf{p},\mathbf{p}'}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{R}}\Gamma_{Is}(\mathbf{p}',i\omega_{n'}|\mathbf{p},i\omega_n)\ , \tag{10}$$

for the lowest Matsubara frequencies $\omega_n=\omega_{n'}=\pi T$. Figure 4 shows Monte Carlo data on $\Gamma_{Is}(\mathbf{R})$ as a function of $\mathbf{R}$ for $T=0.25t$. At $\mathbf{R}=0$, as expected, Γ_{Is} is strongly repulsive, but for an electron pair separated by a near-neighbor distance Γ_{Is} is attractive. As the pair separation $\mathbf{R}$ increases further, Γ_{Is} oscillates in sign and its magnitude decreases rapidly, reflecting the short-range nature of the spin-fluctuation-mediated interaction. For energy transfers which are large compared to the spin-fluctuation energy scale, the on-site interaction reduces to the bare repulsion U. The oscillatory spatial structure of the interaction shown in Fig. 4 has the character of a giant Friedel oscillation. Pairing correlations with the proper space-time structure can avoid the large on-site repulsion while taking advantage of the near-neighbor attraction. Thus, for example, the interaction Γ_{Is} is attractive in the $d_{x^2-y^2}$ channel.

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[12]In NMR calculations (Ref. 13) we have used a random-phase-approximation parametrization, $\chi=\chi_0/(1-\bar{U}\chi_0)$, of the Monte Carlo χ, in order to have a simple form that could be calculated on large lattices at lower temperatures. Here χ_0 is the noninteracting susceptibility, which neglects the single-particle self-energy effects, and $\bar{U}$ is adjusted to $2t$. However, if one were to include the self-energy effects on the irreducible magnetic susceptibility, then we find that it is necessary to use $\bar{U}\simeq 3.2t$ instead of $2t$ in fitting the Monte Carlo (Ref. 11).
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