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Bethe-Salpeter eigenvalues and amplitudes for the half-filled two-dimensional Hubbard model

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Monte Carlo simulations are used to determine the eigenvalues and eigenfunctions of the particle-hole and particle-particle Bethe-Salpeter equations for 8×8 half-filled Hubbard lattice with $U/t=4$ and $U/t=8$. In the particle-hole channel, the dominant eigenvalue corresponds to the $\mathbf{Q}=(\pi,\pi)$ antiferromagnetic correlations. In the particle-particle channel the amplitude of the leading low-temperature eigenvalue is an even-frequency $d_{x^2-y^2}$ singlet. Odd-frequency p-wave-singlet and s-wave-triplet amplitudes are also found.

The nature and interplay of the antiferromagnetic and pairing correlations in the two-dimensional Hubbard model near half-filling remain open questions.[1] In the Hubbard model, the electrons responsible for the antiferromagnetic fluctuations are also the electrons that pair. Thus one would like to examine the particle-hole spin fluctuation and the particle-particle pairing channels on an equal footing. In order to do this we have carried out Monte Carlo calculations of the two-fermion scattering vertex on an 8×8 half-filled two-dimensional Hubbard lattice with

$$H=-t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_{i}(n_{i\uparrow}-\tfrac{1}{2})(n_{i\downarrow}-\tfrac{1}{2}) \ . \tag{1}$$

Here $c_{i\sigma}^{\dagger}$ creates an electron of spin σ on site i, t is a near-neighbor hopping amplitude, and U is the onsite Coulomb repulsion. Equation (1) is written in a particle-hole symmetric form appropriate for a half-filled band. Viewed in the particle-hole channel with center-of-mass momentum $\mathbf{Q}=(\pi,\pi)$, the two-fermion vertex provides direct information on the antiferromagnetic correlations. Viewed in the $\mathbf{q}=(0,0)$ center-of-mass particle-particle channel, it provides information on the nature of the pairing correlations. Here, combining Monte Carlo results for the two-fermion vertex with Monte Carlo calculations of the single-fermion Green's function, we determine the eigenvalues and amplitudes for the $\mathbf{Q}=(\pi,\pi)$ particle-hole and the $\mathbf{q}=(0,0)$ particle-particle Bethe-Salpeter equations. As the temperature is lowered, the dominant eigenvalue, which approaches 1 as T goes to zero, occurs in the particle-hole channel. This signals the formation of the zero-temperature antiferromagnetic phase of the half-filled system. In the particle-particle channel, which describes intermediate states doped with two additional fermions,[2] the dominant eigenvalue at low temperatures is associated with a singlet $d_{x^2-y^2}$ even-frequency amplitude. Additional eigenvalues with odd-frequency pairing amplitudes are also found.

At half-filling, there are no fermion determinantal sign problems,[3] and it is straightforward to calculate the one- and two-fermion propagators,

$$G(x_2,x_1)=-\langle T_\tau c_\sigma(x_2)c_\sigma^{\dagger}(x_1)\rangle \tag{2}$$

and

$$G_2(x_4,x_3,x_2,x_1)=-\langle T_\tau c_{\sigma_4}(x_4)c_{\sigma_3}(x_3)c_{\sigma_2}^{\dagger}(x_2)c_{\sigma_1}^{\dagger}(x_1)\rangle \ . \tag{3}$$

Here $x_l=(l,\tau_l)$ and T_τ is the usual τ-ordering operator. Fourier transforming on both the space- and imaginary-time variables provides information in momentum $\mathbf{p}$ and Matsubara frequency $\omega_n=(2n+1)\pi T$. From the single-particle propagator, Eq. (2), one obtains $G(p)$, and from the two-particle propagator, Eq. (3), $G_2(p_4,p_3,p_2,p_1)$. Here p stands for $(\mathbf{p},i\omega_n)$ and σ.

Given the one- and two-fermion Green's functions, one can obtain the two-fermion scattering vertex Γ from

$$G_2(p_4,p_3,p_2,p_1)=-\delta_{p_1,p_4}\delta_{p_2,p_3}G(p_1)G(p_2)+\frac{T}{N}\delta_{p_1+p_2,p_3+p_4}G(p_4)G(p_3)\Gamma(p_4,p_3,p_2,p_1)G(p_2)G(p_1) \ . \tag{4}$$

With Γ and G one can solve the t-matrix equations represented diagrammatically in Fig. 1 to obtain[4] the irreducible particle-hole vertex $\overline{\Gamma}_{\rm ph}(p|p')$ for a center-of-mass momentum $\mathbf{Q}=(\pi,\pi)$ and the irreducible particle-particle vertex $\overline{\Gamma}_{\rm pp}(p|p')$ for zero center-of-mass momentum. Then, using these, one has the Bethe-Salpeter equations[5] for the particle-hole channel,

$$-\frac{T}{N}\sum_{p'}\overline{\Gamma}_{\rm ph}(p|p')G_\uparrow(p'+Q)G_\downarrow(p')\psi_\alpha(p')=\lambda_\alpha\psi_\alpha(p) \tag{5}$$

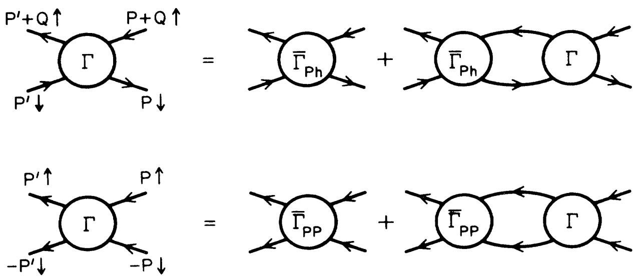

FIG. 1. The particle-hole and particle-particle t-matrix equations. Here the lines represent dressed single-particle propagators and $\mathbf{Q}=(\pi,\pi)$. Γ is the two-fermion scattering vertex, and $\bar{\Gamma}_{ph}$ and $\bar{\Gamma}_{pp}$ are the irreducible particle-hole and particle-particle vertices, respectively.

and the particle-particle channel,

$$-\frac{T}{N}\sum_{p'}\bar{\Gamma}_{pp}(p|p')G_{\uparrow}(p')G_{\downarrow}(-p')\phi_{\alpha}(p')=\lambda_{\alpha}\phi_{\alpha}(p) \ . \quad (6)$$

Here, as before, the sum on p' sums on both the momentum $\mathbf{p}'$ and the Matsubara frequencies $\omega_{n'}=(2n'+1)\pi T$. The upper limit to the Matsubara frequencies that can be obtained is set by the discrete time interval $\Delta\tau$ used in the Monte Carlo simulation. Here we used $\Delta\tau=0.125$ and a corresponding frequency cutoff of order the bandwidth $8t$.

In Figs. 2(a) and 2(b) we have plotted the leading eigenvalues versus temperature for $U=4t$ and $U=8t$, respectively. These results were obtained for a half-filled 8×8 lattice. If an eigenvalue reaches 1, this implies an instability in the scattering response. At half-filling, the dominant response, the solid circles in Fig. 2, occurs in the particle-hole $\mathbf{Q}=(\pi,\pi)$ channel, reflecting the strong antiferromagnetic fluctuations. The open symbols show the behavior of three of the leading particle-particle eigenvalues of Eq. (6). Comparing the results shown in Figs. 2(a) and 2(b), one can see that increasing U from $4t$ to $8t$ has a dramatic effect on the size of the particle-particle eigenvalues at higher temperatures. For example, at a temperature $T=0.25t$, the $d_{x^2-y^2}$ wave eigenvalue increases by almost a factor of 3 when U is changed from $4t$ to $8t$. In addition, it changes from the second leading eigenvalue to the leading one.

The momentum and frequency dependence of the leading antiferromagnetic eigenvalue, $\psi_s(\mathbf{p},i\omega_n)$ are shown[6] in Figs. 3(a) and 3(b) for an 8×8 lattice with $U=8t$ and $T=0.25t$. We see that ψ_s is essentially a constant function of the relative momentum, corresponding to a magnetization operator of the form

$$m_{\mathbf{Q}}^{+}=\frac{1}{\sqrt{N}}\sum_{\mathbf{p}}g(\mathbf{p})c^{\dagger}_{\mathbf{p}+\mathbf{Q}\uparrow}c_{\mathbf{p}\downarrow} \ , \quad (7)$$

with $g(\mathbf{p})\simeq1$. However, it has structure in ω_n implying that retardation plays a role in the antiferromagnetic correlations. Including retardation, the magnetization eigenoperator would have the form

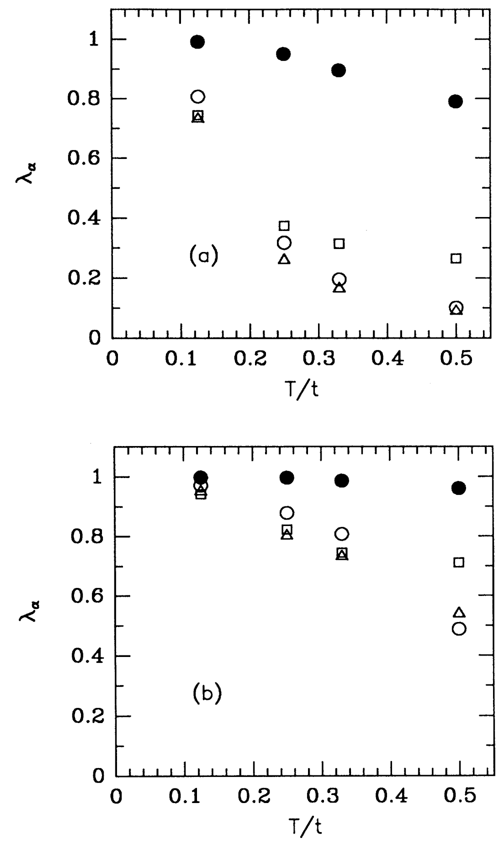

FIG. 2. Eigenvalues of the Bethe-Salpeter equations vs T for (a) $U=4t$ and (b) $U=8t$ for an 8×8 half-filled lattice. The solid points are for the $\mathbf{Q}=(\pi,\pi)$ antiferromagnetic particle-hole eigenvalue of Eq. (3). The open symbols denote the eigenvalues of the $\mathbf{q}=(0,0)$ particle-particle Bethe-Salpeter Eq. (4) with (○) corresponding to the singlet $d_{x^2-y^2}$ even-frequency amplitude, (△) to a singlet, odd-frequency p-wave amplitude, and (□) to a triplet, s-wave odd-frequency amplitude.

$$m_{\mathbf{Q}}^{+}(\tau)=\int_{-\beta}^{\beta}\frac{d\tau'}{2\beta}\frac{1}{\sqrt{N}}\sum_{\mathbf{p},i\omega_n}e^{-i\omega_n\tau'}\psi(\mathbf{p},i\omega_n) \times Tc^{\dagger}_{\mathbf{p}+\mathbf{Q}\uparrow}(\tau+\tau')c_{\mathbf{p}\downarrow}(\tau) \ . \quad (8)$$

As seen in Fig. 3(b), $\psi(\mathbf{p},i\omega_n)$ remains finite over the entire bandwidth implying that the usual magnetization operator $(1/\sqrt{N})\sum_{\mathbf{p}}c^{\dagger}_{\mathbf{p}+\mathbf{Q}\uparrow}c_{\mathbf{p}\downarrow}$ has a good overlap with the eigenoperator. We also find additional eigenfunctions with smaller eigenvalues. Some of these eigenfunctions are odd in ω_n just as some of the particle-particle eigenfunctions discussed below. However, all of the other eigenvalues are small compared to the dominant antiferromagnetic one.

The momentum and frequency dependence of the leading particle-particle Bethe-Salpeter amplitudes $\phi_d(\mathbf{p},i\omega_n)$, $\phi_p(\mathbf{p},i\omega_n)$, and $\phi_s(\mathbf{p},i\omega_n)$ are shown in Figs. 4(a) and 4(b). At low temperatures, the leading pairing eigenfunction has $d_{x^2-y^2}$ symmetry in momentum space and is even in frequency. The next leading eigenfunction has p_x (or p_y) symmetry in momentum and is odd in frequency, while the next one has s symmetry in momentum and is also odd in frequency. The p_x (p_y) eigenfunctions correspond to the singlet odd-frequency gap proposed by Balatsky and Abrahams,[7] while the s-state triplet corresponds to the odd-frequency gap discussed by Brezinskii.[8] At higher temperatures, the leading eigenvalue in the particle-particle channel corresponds to an odd-frequency s-wave triplet. Comparing Figs. 4(b) and 3(b), one also observes that the pairing eigenvalues decay faster in frequency than the leading magnetic eigenvalue. Thus, as expected, retardation plays a much more important role in the pairing channel. In fact, the odd-frequency amplitudes imply that the equal-time two-fermion part of the corresponding pair-field operator vanishes. Thus retardation is essential for the odd-frequency fluctuations. Note that the effective pair-field eigenoperator has the form of Eq. (8) with $\psi(\mathbf{p},i\omega_n)$ replaced by $\phi_\alpha(\mathbf{p},i\omega_n)$ and $c^\dagger_{\mathbf{p}+\mathbf{Q}\uparrow}(\tau+\tau')c_{\mathbf{p}\downarrow}(\tau)$ replaced by $c^\dagger_{\mathbf{p}\uparrow}(\tau+\tau')c^\dagger_{-\mathbf{p}\downarrow}(\tau)$.

We interpret these results as evidence that two holes (or electrons) added to a half-filled 8×8 Hubbard lattice

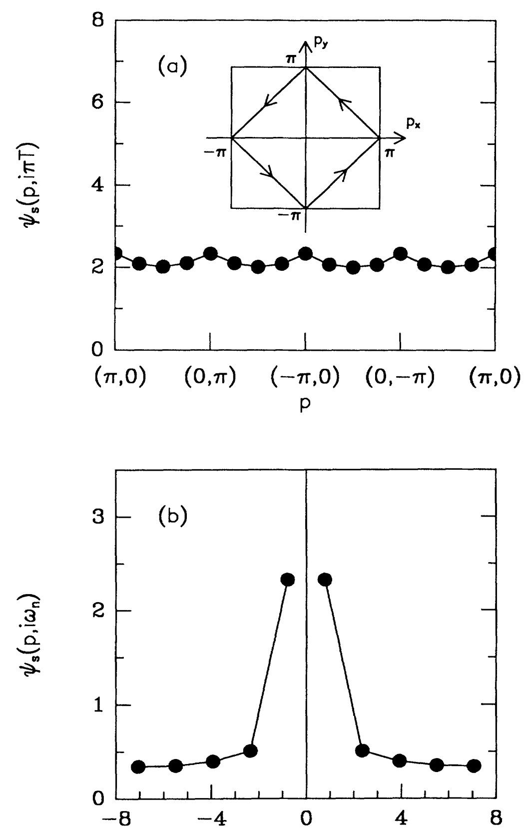

FIG. 3. Monte Carlo results for the leading magnetic eigenfunction $\psi_s(\mathbf{p},i\omega_n)$ on an 8×8 lattice with $U=8t$ and $T=0.25t$. (a) Momentum structure of $\psi_s(p,i\pi T)$. Here $\mathbf{p}$ is taken along the path shown in the inset. (b) Frequency structure of $\psi_s(\mathbf{p},i\omega_n)$ for $\mathbf{p}=(\pi,0)$.

lead to a state with strong pairing correlations. The fact that at low temperatures, the pair eigenfunction with the largest eigenvalue has $d_{x^2-y^2}$ symmetry is consistent with previous exact diagonalization[9] and Monte Carlo studies[10] of 4×4 lattices. In these calculations the ground state of the half-filled 4×4 Hubbard model was found to

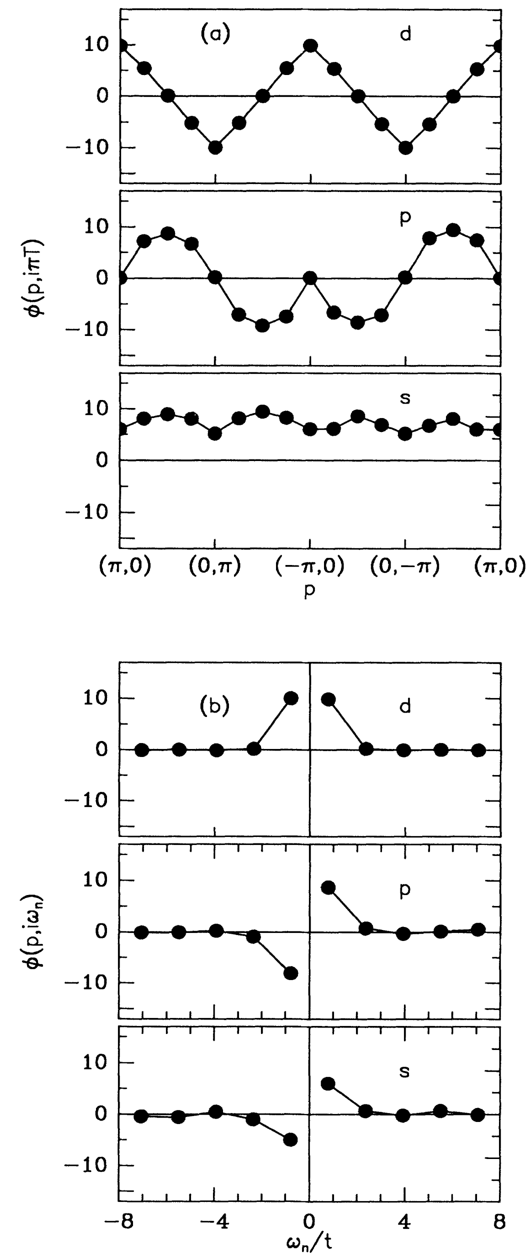

FIG. 4. Monte Carlo results for the leading eigenfunctions in the pairing channel, $\phi_d(\mathbf{p},i\omega_n)$, $\phi_p(\mathbf{p},i\omega_n)$, and $\phi_s(\mathbf{p},i\omega_n)$, on an 8×8 lattice with $U=8t$ and $T=0.25t$. (a) Momentum structure of the leading eigenfunction for $\omega_n=\pi T$. Here $\mathbf{p}$ is taken along the path shown in the inset of Fig. 3(a). (b) Frequency structure of the leading eigenfunctions. Here $\phi_d(\mathbf{p},i\omega_n)$ and $\phi_s(\mathbf{p},i\omega_n)$ are shown for $\mathbf{p}=(\pi,0)$, and $\phi_p(\mathbf{p},i\omega_n)$ is shown for $\mathbf{p}=(\pi/2,\pi/2)$.

have s-wave symmetry, while for $U \gtrsim 3t$, the ground state of the system with two electrons removed (or added) was found to have $d_{x^2-y^2}$ symmetry. Thus the pair-field operator connecting these two states must have $d_{x^2-y^2}$ symmetry. In addition, previous Monte Carlo simulations[11] in which pair-field susceptibility with and without the two-particle vertex were calculated, showed that there was an attractive interaction in the $d_{x^2-y^2}$ channel. However, the results reported here differ from previous Monte Carlo calculations in that by studying the Bethe-Salpeter equations, we have allowed the system to select the internal momentum, frequency, and spin structure of the dominant pairing correlations rather than imposing this structure by a particular choice for the pair-field operator. Furthermore, by studying the case where two fermions are added to a half-filled band, we have been able to run the Monte Carlo simulations at significantly lower temperatures and larger values of U than can be achieved in simulations carried out away from half-filling.

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[2]Starting with a half-filled 8×8 lattice and adding two fermions corresponds to a doping $\delta = 66/64 - 1 \cong 0.03$.

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[5]Equivalent forms for these Bethe-Salpeter equations, which directly involve only G and G_2, can be written as

$$-\sum_p{}' \frac{G_2(p+Q,p,p',p'+Q)}{G(p+Q)G(p)}\psi_\alpha(p') = \frac{1}{1-\lambda_\alpha}\psi_\alpha(p)$$

and

$$-\sum_p{}' \frac{G_2(p,-p,-p',p')}{G(p)G(-p)}\phi_\alpha(p') = \frac{1}{1-\lambda_\alpha}\phi_\alpha(p) \; .$$

Note that λ_α, ψ_α, and ϕ_α are the same eigenvalues and eigenfunctions that appear in Eqs. (5) and (6).

[6]The eigenfunctions are normalized such that $(T/N)\sum_p \psi_\alpha^2(p) = 1$.

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