PAIRING MECHANISM IN THE TWO–DIMENSIONAL HUBBARD MODEL

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Here we discuss Quantum Monte Carlo results for the magnetism susceptibility, single–particle spectral weight and the irreducible particle–particle interaction vertex of the two–dimensional Hubbard model. In the doped system, as the temperature is lowered below $J = 4t^2/U$, short–range antiferromagnetic correlations develop. These lead to a narrow low–energy quasiparticle band with a large Fermi surface and a particle–particle vertex which increases at large momentum transfer, which favor $d_{x^2−y^2}$–pairing.

A variety of experiments on the high $T_c$ cuprates can be interpreted in terms of a gap with dominant $d_{x^2−y^2}$ symmetry [1]. However, the implications of this with respect to the nature of the underlying pairing mechanism remains an open question. Here we review some results which have been obtained for the two–dimensional Hubbard model, which has been found to exhibit $d_{x^2−y^2}$–like pairing fluctuations. Our aim is to examine in this particular case the structure of the quasiparticle spectrum and the interaction in order to gain insight into the mechanism which leads to $d_{x^2−y^2}$ pairing correlations in this model.

The two-dimensional Hubbard Hamiltonian provides an approximate model of a CuO$_2$ layer:

$$H = -t \sum_{\langle ij \rangle, s} (c_{is}^\dagger c_{js} + c_{js}^\dagger c_{is}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Here $c_{is}^\dagger$ creates an electron of spin $s$ on site $i$, and $n_{is} = c_{is}^\dagger c_{is}$ is the occupation number for spin $s$ on site $i$. The one–electron transfer between near–neighbor sites is $t$, and $U$ is an onsite Coulomb energy. The bare energy scale is set by the bandwidth $8t$ and the effective Coulomb interaction $U$, which are both of order electron volts. Near half–filling, electrons on neighboring sites tend to align antiferromagnetically so as to lower their energy by the exchange interaction $J = 4t^2/U$. This interaction is of order a tenth of an electron volt and, as we will see, sets the energy, or temperature scale, below which antiferromagnetic (AF) correlations, the low–energy structure in the single–particle spectral weight, and the pairing interaction develop.

While Monte Carlo [2] and Lanczos [3] calculations for a $4 \times 4$ lattice find that two holes added to the half–filled Hubbard ground state form a $d_{x^2−y^2}$ bound state, and density matrix renormalization group calculations [4] find that $d_{x^2−y^2}$–like pairs are formed on two–leg Hubbard ladders, it is not known what happens for the two–dimensional Hubbard model. It is possible that on an energy scale of order $J/10$, a $d_{x^2−y^2}$ superconducting state forms. However, this may well require modifications of the model, such as an additional near–neighbor $\Delta J S_i \cdot S_j$ term or possibly a next–near–neighbor hopping $t'$. Nevertheless, it is known that as the temperature is reduced below $J$, $d_{x^2−y^2}$ pairing correlations develop in the doped two–dimensional Hubbard model, and here we will examine why this happens.

At half–filling, $\langle n_{i\uparrow} + n_{i\downarrow} \rangle = 1$, the 2D Hubbard model develops long–range antiferromagnetic order as the temperature goes to zero. In the doped case, strong short–range AF correlations develop as the temperature decreases below $J$. This is clearly seen in the temperature dependence of the wave vector dependent magnetic susceptibility

$$\chi(\mathbf{q}) = \frac{1}{N} \sum_{\ell} \int_0^\beta d\tau \langle m_{i+\ell}^\dagger(\tau) m_{i}^\dagger(0) \rangle e^{-i\mathbf{q} \cdot \mathbf{\ell}}. \quad (2)$$
Here \( m_i^+ = c_i^\dagger c_i \) and \( m_{i+\ell}^{-}(\tau) = e^{i\tau} m_{i+\ell}^{+} e^{-i\tau} \), where \( m_{i+\ell}^{+} \) is the hermitian conjugate of \( m_i^+ \).

Monte Carlo results for \( \chi(q) \) versus \( q \) along the (1,1) axis for an 8 \( \times \) 8 lattice with \( U/t = 4 \) and a filling \( \langle n \rangle = 0.875 \) are shown in Fig. 1(a). As the temperature decreases below \( J = 4t^2/U \), significant short–range dynamic AF correlations evolve. Fig. 1(b) shows the AF correlation length \( \xi_{\text{AF}} \) versus \( T \). Here, \( \xi_{\text{AF}}^{-1} \) is defined as the half–width at half–maximum of \( \chi(q) \).

As these AF correlations develop, the single-particle spectral weight 

\[
A(p, \omega) = -\frac{1}{\pi} \text{Im} \ G(p, i\omega_n \rightarrow \omega + i\delta) \tag{3}
\]

and the density of states \( N(\omega) = \frac{1}{\pi} \sum_p A(p, \omega) \) also change. Figure 2(a) shows \( N(\omega) \) for \( U/t = 8 \) and \( \langle n \rangle = 0.875 \). As the temperature is lowered, a peak appears on the upper edge of the lower Hubbard band.

This peak arises from a narrow quasiparticle band shown in the single–particle spectral weight \( A(p, \omega) \) of Fig. 2 and plotted as the solid curve in Fig. 2(b). As the momentum \( p \) goes towards the \( \Gamma \) point \((0,0)\), we believe that the quasiparticle peak is obscured by the lower Hubbard band because of the resolution of the maximum entropy technique which we have used. Indeed, at the \( \Gamma \) point a separate quasiparticle peak is found from Lanczos exact diagonalization on a 4 \( \times \) 4 lattice. Note that this implies a large hole–like Fermi surface. As clearly evident in the spectral weight shown in Figs. 2(a) and (b), the quasiparticle dispersion is anomalously flat near the \((\pi,0)\) corner. As discussed by various authors, this reflects the influence of the AF correlations on the quasiparticle excitation energy. It is clear that the peak structure in \( N(\omega) \) also arises from the short–range AF correlations and is a many–body effect rather than simply a non–interacting band Van Hove singularity.

Monte Carlo calculations have also been used to determine the singlet irreducible particle–particle vertex \( \Gamma_{1S}(p', -p', p, -p) \) in the zero center–of–mass momentum and energy channel which gives the effective pairing interaction. Here \( p = (p, i\omega_n) \). In Fig. 4(a), \( \Gamma_{1S}(q = p - p') \) is plotted for \( q \) along the (1,1) direction and \( i\omega_n = i\omega_{n'} = i\pi T \), corresponding to zero Matsubara energy transfer. Comparing Figs. 1(a) and 4(a), one clearly sees that the structure of the interaction
Figure 2: (a) Evolution of the single-particle density of states with temperature for $U/t = 8$ and $\langle n \rangle = 0.875$. (b) Dispersion of the quasiparticle peak in the spectral weight versus $p$. The solid points mark the low-energy peaks of $A(p, \omega)$ shown in Fig. 3, and the solid curve represents an estimate of the quasiparticle dispersion using these data and Lanczos results for $p$ near $(0,0)$. The broad darkened areas represent the incoherent spectral weight in the upper and lower Hubbard bands. The horizontal dashed line denotes the chemical potential $\mu$.

Figure 3: Single-particle spectral weight along various cuts in the Brillouin zone is shown for $U/t = 8$ and $\langle n \rangle = 0.875$ on a $12 \times 12$ lattice at $T = 0.5t$. 
Figure 4: (a) Singlet irreducible particle–particle vertex for zero energy transfer $\Gamma_{IS}(q, i\omega_n = 0)$ versus $q$ along the (1,1) direction. As the temperature decreases below $J = 4t^2/U$, the strength of the interaction is enhanced at large momentum transfer. Note the similarity to $\chi(q)$ in Fig. 1(a). (b) Temperature dependence of the $d_{x^2-y^2}$ eigenvalue of the Bethe–Salpeter equation. These results are for $U/t = 4$ and $\langle n \rangle = 0.875$.

and $\chi(q)$ are similar, both reflecting the development of the AF correlations as $T$ is reduced below $J$.

Given the Monte Carlo results for the irreducible particle–particle vertex $\Gamma_{IS}(p', -p', p, -p)$ in the zero energy and center–of–mass momentum channel, and the single–particle Green’s function $G(p, i\omega_n)$, the Bethe–Salpeter equation for the particle–particle channel is

$$\lambda_\alpha \phi_\alpha(p) = -\frac{T}{N} \sum_{p'} \Gamma_{IS}(p, -p, p', -p') |G(p')|^2 \phi_\alpha(p').$$  (4)

Here, the sum on $p'$ is over both $p'$ and $\omega_n$. In the parameter regime that the Monte Carlo simulations are carried out, the leading singlet eigenvalue is in the $d_{x^2-y^2}$ channel. Fig. 4(b) shows the temperature dependence of the $d_{x^2-y^2}$ eigenvalue.

The development of both the low–energy quasiparticle dispersion and the peak in the singlet particle–particle vertex at large momentum transfers arises from the growth of short–range AF correlations as $T$ decreases below $J$. As is known [5], for the large Fermi surface associated with the observed quasiparticle dispersion, a particle–particle vertex which increases at large momentum transfer favors $d_{x^2-y^2}$ pairing. Note that the tendency for $d_{x^2-y^2}$ pairing does not require a particularly sharp or narrow peak in $\Gamma_{IS}(q)$ for $q = (\pi, \pi)$, but rather simply sufficient weight at large momentum transfers. Thus it is the strong short–range AF correlations which lead to the formation of $d_{x^2-y^2}$ pairing correlations in the Hubbard model.

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