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$d_{x^2-y^2}$ Pairing correlations in the Hubbard ladder

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Abstract

We study the strength and the temperature scale of the $d_{x^2-y^2}$ pairing correlations in the two-leg Hubbard ladder using quantum Monte Carlo (QMC) simulations. In particular, we present QMC results on the solution of the Bethe–Salpeter equation for the $d_{x^2-y^2}$-wave BCS channel. These data show that, at sufficiently low temperatures, there are strong $d_{x^2-y^2}$ pairing correlations in the Hubbard ladder.
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The pairing correlations in the two-leg Hubbard model have been studied using various techniques of many-body physics [1–5]. In particular, the DMRG calculations found that the $d_{x^2-y^2}$ pairing correlations are strongest near half-filling for Coulomb repulsion in the intermediate coupling regime and for hopping anisotropy $t_\perp/t \approx 1.5$ [4]. In fact, the two-leg Hubbard ladder is probably the only model where it is known from exact calculations that the pairing correlations get enhanced by turning on an onsite Coulomb repulsion in the ground state [3,4]. Hence, it is important to know the characteristic temperature scale and the strength of the pairing correlations in this model, which is the purpose of this paper.

Here, we present QMC results on the $d_{x^2-y^2}$ eigenvalue λ_d of the Bethe–Salpeter equation. In particular, we study the dependence of λ_d on the temperature T, doping and the Coulomb repulsion U. We show that, at sufficiently low T, there are strong $d_{x^2-y^2}$ pairing correlations near half-filling. In addition, we present QMC results on the magnetic susceptibility in the same parameter regime.

The two-leg Hubbard model is defined by

$$H = -t\sum_{i,\lambda,\sigma}(c^\dagger_{i,\lambda,\sigma}c_{i+1,\lambda,\sigma} + \text{h.c.}) - t_\perp\sum_{i,\sigma}(c^\dagger_{i,1,\sigma}c_{i,2,\sigma} + \text{h.c.}) + U\sum_{i,\lambda} n_{i,\lambda,\uparrow}n_{i,\lambda,\downarrow} - \mu\sum_{i,\lambda,\sigma} n_{i,\lambda,\sigma}, \quad (1)$$

where t ($t_\perp$) is the hopping parameter parallel (perpendicular) to the chains. The operator $c^\dagger_{i,\lambda,\sigma}$ ($c_{i,\lambda,\sigma}$) creates (annihilates) an electron of spin σ at site i of chain λ, and $n_{i,\lambda,\sigma} = c^\dagger_{i,\lambda,\sigma}c_{i,\lambda,\sigma}$ is the electron occupation number. As usual, U is the Coulomb repulsion, and μ is the chemical potential. In addition, periodic boundary conditions are used along the chains. In the ground state and for $U = 4t$, the $d_{x^2-y^2}$ pairing correlations are most enhanced near half-filling for $t_\perp \approx 1.6t$ [4]. When $U = 8t$, this occurs for $t_\perp \approx 1.4t$. Here, the QMC data will be presented using these parameter sets for a 2×16 lattice.

The Bethe–Salpeter equation in the BCS channel is given by

$$\frac{\lambda_\alpha}{1-\lambda_\alpha}\phi_\alpha(p) = -\frac{T}{N}\sum_{p'}\Gamma(p|p')|G(p')|^2\phi_\alpha(p') \quad (2)$$

with $p = (\mathbf{p}, i\omega_n)$ and $\omega_n = (2n+1)\pi T$. Here, $\Gamma(p'|p)$ is the reducible particle–particle interaction in the BCS channel

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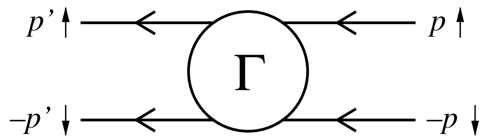

Fig. 1. Feynman diagram for the reducible particle–particle interaction $\Gamma(p'|p)$ in the BCS channel.

illustrated in Fig. 1, $G(p)$ is the single-particle Green's function, λ_α is the irreducible eigenvalue in channel α, and $\phi_\alpha(p)$ is the corresponding eigenvalue. We have calculated $\Gamma(p'|p)$ and $G(p)$ with the QMC technique [6]. For a three-dimensional infinite system, when the maximum λ_α reaches 1, this signals a BCS instability to a state where the pair-wave function at T_c has the form of the corresponding eigenfunction $\phi_\alpha(\mathbf{p}, i\omega_n)$.

At low temperatures, the maximum λ_α of the Bethe–Salpeter equation corresponds to an eigenfunction $\phi_d(\mathbf{p}, i\omega_n)$ which has $d_{x^2-y^2}$ type of symmetry [5]. The T dependence of λ_d is shown in Fig. 2a for $U = 4t$ and $t_\perp = 1.6t$. Here, it is seen that, as T decreases, λ_d grows monotonically reaching 0.75 at $T = 0.1t$ for $\langle n\rangle = 0.94$. Upon doping to $\langle n\rangle = 0.875$, λ_d decreases. Also shown in Fig. 2b is λ_d for $U = 8t$ and $t_\perp = 1.4t$. At the temperatures where these calculations were performed, we find that λ_d is larger for $U = 8t$.

Next, Fig. 2c and d display QMC results on the T dependence of the AFM susceptibility $\chi(\mathbf{q} = (\pi,\pi))$ for the same parameters as in Fig. 2a and b, respectively. Here $\chi(\mathbf{q})$ is defined by

$$\chi(\mathbf{q}) = \int_0^\beta d\tau \langle m^-_{\mathbf{q}}(\tau) m^+_{\mathbf{q}}(0)\rangle \qquad (3)$$

with $m^+_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{p}} c^\dagger_{\mathbf{p}+\mathbf{q}\uparrow} c_{\mathbf{p}\downarrow}$, $m^-_{\mathbf{q}} = (m^+_{\mathbf{q}})^\dagger$ and $m^-_{\mathbf{q}}(\tau) = e^{H\tau} m^-_{\mathbf{q}} e^{-H\tau}$. In Fig. 2c and d, we observe the development of the AFM correlations, as T decreases. However, as $T \to 0$, $\chi(\mathbf{q} = (\pi,\pi))$ will saturate, since the ground state of the Hubbard ladder has short-range AFM correlations. These figures also show that, upon doping at low T, λ_d decays slower than $\chi(\mathbf{q} = (\pi,\pi))$. In addition, we observe that the large values of λ_d seen in Fig. 2a and b do not necessarily require strongly enhanced AFM correlations.

In this paper, we have investigated the $d_{x^2-y^2}$ pairing correlations in the Hubbard ladder by presenting QMC data on the T, U/t and the doping dependence of the $d_{x^2-y^2}$-wave eigenvalue of the Bethe–Salpeter equation. In addition, we have presented QMC data on the AFM susceptibility in the same parameter regime. These data show that the $d_{x^2-y^2}$ pairing correlations in the Hubbard ladder are strong for certain values of the model parameters.

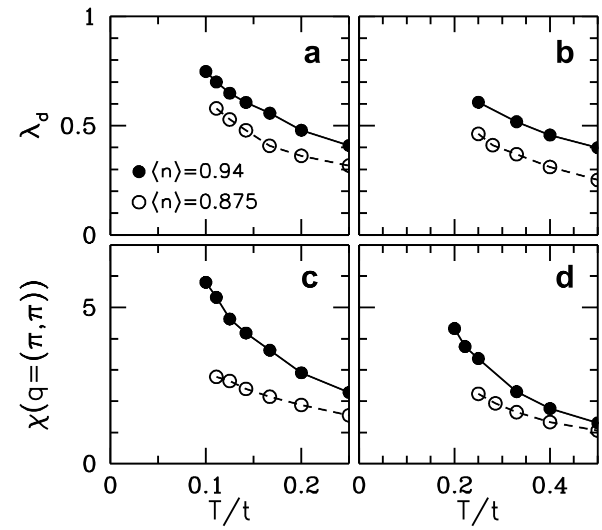

Fig. 2. $d_{x^2-y^2}$-Wave irreducible eigenvalue λ_d of the Bethe–Salpeter equation versus T (a) for $U = 4t$ and $t_\perp = 1.6t$, and (b) for $U = 8t$ and $t_\perp = 1.4t$. Antiferromagnetic susceptibility $\chi(\mathbf{q} = (\pi,\pi))$, in units of t^{-1}, versus T (c) for $U = 4t$ and $t_\perp = 1.6t$, and (d) for $U = 8t$ and $t_\perp = 1.4t$.

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