RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 47, NUMBER 10 1 MARCH 1993-II

Rapid Communications

Rapid Communications are intended for the accelerated publication of important new results and are therefore given priority treatment both in the editorial office and in production. A Rapid Communication in **Physical Review B** *should be no longer than four printed pages and must be accompanied by an abstract. Page proofs are sent to authors.*

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

N. Bulut
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

D. J. Scalapino
Department of Physics, University of California, Santa Barbara, California 93106

S. R. White
Department of Physics, University of California, Irvine, California 92717
(Received 29 December 1992)

The irreducible particle-particle interaction Γ_I of the two-dimensional Hubbard model is calculated by quantum Monte Carlo simulations. The Bethe-Salpeter equation for the pair-wave function is then solved using the Monte Carlo data for Γ_I and the single-particle Green's function. The dominant pairing correlations in the intermediate-coupling regime and at small dopings are discussed.

The nature and extent of the pairing correlations in a two-dimensional Hubbard model doped near half filling remains an open question. Diagrammatic calculations based upon the exchange of spin fluctuations suggested the possibility of $d_{x^2-y^2}$-wave pairing.[1–3] Spin bag models,[4] Gutzwiller variational calculations,[5] and $1/N$ expansions[6] find $d_{x^2-y^2}$ pairing or in some cases extended s-wave or $(d+is)$-wave pairing. Monte Carlo simulations of various pair-field susceptibilities[7,8] have so far only found evidence for short-range $d_{x^2-y^2}$ and extended s-wave correlations. However, the pair-field operators which have been studied by simulation were constructed using equal-time bare fermion operators which may have only a limited overlap with the dressed pair field.[9] Or worse yet, these pair fields might not have the correct symmetry, particularly if this involves the relative time dependence of the pair-field operators. In order to obtain more detailed information about the space and imaginary-time structure of the pairing correlations, we have carried out Monte Carlo calculations of the irreducible particle-particle interaction Γ_I. Using this interaction along with Monte Carlo results for the one-electron Green's function, we then solve the particle-particle Bethe-Salpeter equation and determine the strength of the eigenvalues and the $(\mathbf{p},i\omega_n)$ structure of the leading pair-field eigenfunctions. We find at high temperatures, or order $J\sim 4t^2/U$, that the dominant pairing correlations occur in an odd-frequency, s-wave triplet channel. However, as the temperature is lowered, the strength in the even-frequency $d_{x^2-y^2}$ and the odd-frequency p_x (or p_y) singlet channels grows the most rapidly.

Using quantum Monte Carlo simulations we have calculated the two-particle Green's function

$$\Lambda(x_4,x_3|x_1,x_2)=-\langle T_\tau c_\uparrow(x_4)c_\downarrow(x_3)c_\downarrow^\dagger(x_2)c_\uparrow^\dagger(x_1)\rangle \ . \tag{1}$$

Here $c_\sigma^\dagger(x_i)$ with $x_i=(\mathbf{x}_i,\tau_i)$ creates an electron of spin σ at site $\mathbf{x}_i$ and imaginary time τ_i. T_τ is the usual τ-ordering operator. Fourier transforming on both the space and imaginary time variables allows us to determine

$$\begin{aligned}\Lambda(p',k'|p,k)=&-\delta_{p,p'}\delta_{k,k'}G_\uparrow(p)G_\downarrow(k)\\&+\frac{T}{N}\delta_{k',p+k-p'}G_\uparrow(p')G_\downarrow(k')\\&\times\Gamma(p',k'|p,k)G_\uparrow(p)G_\downarrow(k)\ ,\end{aligned} \tag{2}$$

from which one can obtain the reducible particle-particle vertex $\Gamma(p',k'|p,k)$. Here $p=(\mathbf{p},i\omega_n)$ and $G_\sigma(p)$ is the single-particle Green's function. We will calculate the particle-particle interaction in the zero center-of-mass momentum and energy channel, hence we set $k=-p$ and $k'=-p'$. In order to obtain the irreducible particle-particle vertex Γ_I, we use the Monte Carlo results for Γ and G to solve the t-matrix equation for Γ_I,

$$\begin{aligned}\Gamma(p'|p)=&\Gamma_I(p'|p)\\&-\frac{T}{N}\sum_k\Gamma_I(p'|k)G_\uparrow(k)G_\downarrow(-k)\Gamma(k|p)\ .\end{aligned} \tag{3}$$

Here $\Gamma(p'|p)$ is used as a short notation for $\Gamma(p',-p'|p,-p)$. In this calculation, Matsubara frequencies ω_n up to the bandwidth $8t$ were kept. Runs with the cutoff at $12t$ gave similar results. This procedure is essentially the opposite one from the usual diagrammatic approach in which an irreducible vertex such as Γ_I

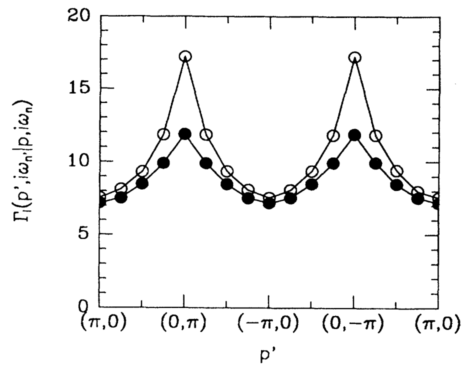

FIG. 1. Monte Carlo results for the irreducible particle-particle interaction, $\Gamma_I(\mathbf{p}', i\omega_{n'}|\mathbf{p}, i\omega_n)$, for $U=4t$, $\langle n\rangle \sim 0.87$, and $\omega_n=\omega_{n'}=\pi T$ on an 8×8 lattice at $T=0.50t$ (solid circles) and $T=0.25t$ (open circles). Here $\mathbf{p}'$ is taken along the path shown in Fig. 2, and $\mathbf{p}$ is kept fixed at $(\pi,0)$. The error bars are of order twice the size of the circles.

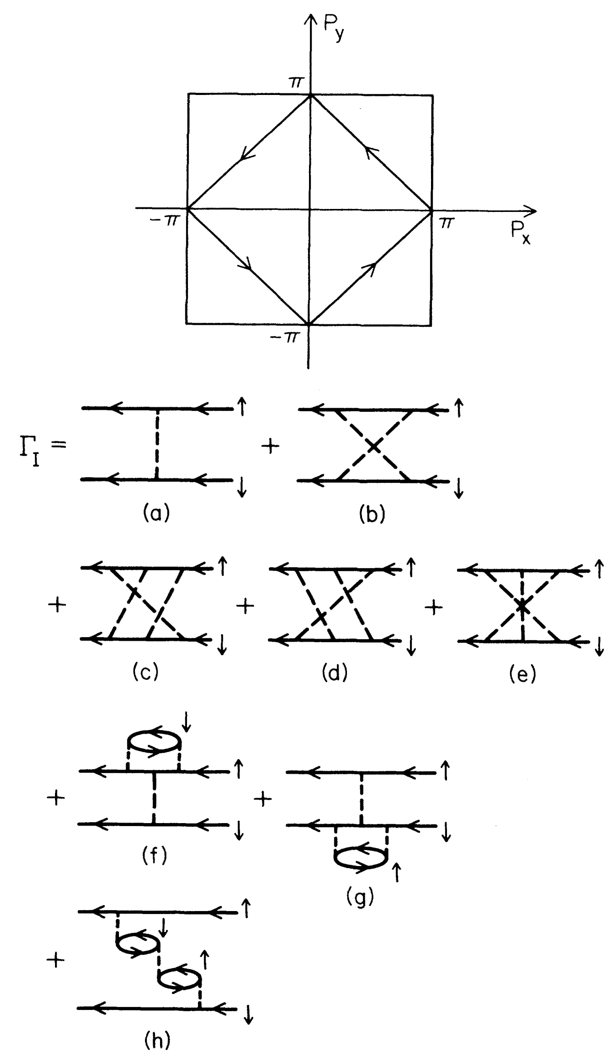

FIG. 2. The upper part of this figure shows the path $\mathbf{p}'$ follows in Figs. 1 and 3. The lower portion shows the Feynman graphs for Γ_I through third order.

is selected and then Γ is calculated from Eq. (3).

We first present Monte Carlo results obtained for Γ_I on an 8×8 lattice[10] with $U=4t$ and an average density $\langle n\rangle \sim 0.87$. In Fig. 1, the irreducible interaction $\Gamma_I(p'|p)$ is plotted as a function of $\mathbf{p}'$ for $\omega_n=\omega_{n'}=\pi T$ at $T=0.50t$ (solid circles) and $0.25t$ (open circles). In this plot $\mathbf{p}'$ follows the contour shown in Fig. 2, while $\mathbf{p}$ is kept fixed at $(\pi,0)$. We observe that Γ_I peaks at large momentum transfers and the strength of this peak increases as the temperature is lowered. We also find that at (π,π) momentum transfer and $T=0.25t$, $\Gamma_I(p'|p)$ for $\omega_n=\pi T$ and $\omega_{n'}=-\pi T$ is about 50% larger than that for $\omega_n=\omega_{n'}=\pi T$.

To gain further insight into the structure of the irreducible interaction, we have calculated $\Gamma_I(p'|p)$ through third order, keeping the contributions shown in Fig. 2. The results are shown in Fig. 3 with the solid circles for $T=0.50t$ and the open circles for $T=0.25t$. Here the dominant contributions come from graphs (a), (b), and (e) along with (h). Graphs (b) and (e) represent the leading transverse and graph (h) the leading longitudinal spin-fluctuation contributions to the Berk-Schrieffer[11] interaction. Graphs (c) and (d) are negative and can be thought of as reducing the strength of the effective Coulomb interaction which enters (b). The leading vertex corrections (f) and (g) enhance the interaction at small momentum transfer. The structure of the interaction reflects the underlying antiferromagnetic correlations.

In order to determine the structure of the pairing correlations which are produced by the particle-particle interaction Γ_I shown in Fig. 1, we have solved[12] the Bethe-Salpeter equation

$$\lambda_\alpha\phi_\alpha(p) = -\frac{T}{N}\sum_{p'}\Gamma_I(p|p')G_\uparrow(p')G_\downarrow(-p')\phi_\alpha(p') \quad (4)$$

for its eigenfunctions $\phi_\alpha(p)$ and the corresponding eigenvalues λ_α using Monte Carlo data for Γ_I and $G(p)$. As is well known, when the largest λ_α reaches 1, a superconducting instability to a state having the pair-wave function $\phi_\alpha(p)$ occurs. In general, the Bethe-Salpeter equation can have both singlet and triplet solutions corresponding to a pair-wave function that has overall even or odd parity when $p=(\mathbf{p},i\omega_n)$ goes to $(-\mathbf{p},-i\omega_n)$. We

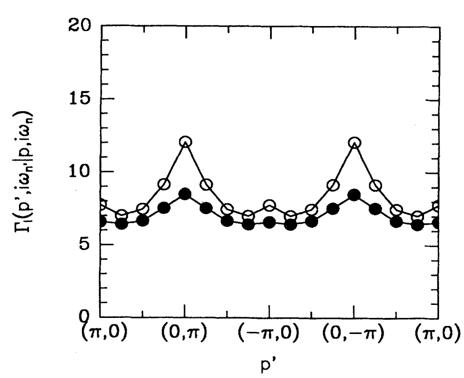

FIG. 3. Third-order perturbation theory results for $\Gamma_I(\mathbf{p}', i\omega_{n'}|\mathbf{p}, i\omega_n)$ for the same parameters as in Fig. 1.

will characterize $\phi_\alpha(\mathbf{p},i\omega_n)$ by its symmetry in momentum and spin space. The usual singlet s and $d_{x^2-y^2}$-wave states are even in frequency and even in momentum, $\phi(\mathbf{p},-i\omega_n)=\phi(\mathbf{p},i\omega_n)$ and $\phi(-\mathbf{p},i\omega_n)=\phi(\mathbf{p},i\omega_n)$, while the usual triplet p_x (or p_y) state is even in frequency and odd when p_x goes to $-p_x$. As discussed by Berezinskii[13] and recently by Balatsky and Abrahams,[14] there can also be odd-frequency pair-wave functions. In this case one could have an odd-frequency s-wave triplet for which $\phi(\mathbf{p},-i\omega_n)=-\phi(\mathbf{p},i\omega_n)$ and $\phi(-\mathbf{p},i\omega_n)=\phi(\mathbf{p},i\omega_n)$, or an odd-frequency p_x (or p_y)-wave singlet with $\phi(\mathbf{p},-i\omega_n)=-\phi(\mathbf{p},i\omega_n)$ and $\phi(-\mathbf{p},i\omega_n)=-\phi(\mathbf{p},i\omega_n)$. In the regime of the Hubbard model that we are studying, we find that the s-wave triplet, and the p and $d_{x^2-y^2}$-wave singlet solutions are dominant.

The four largest eigenvalues for $U=4t$ and $U=8t$ on an 8×8 lattice are given in Table I. The momentum and the frequency dependences of the corresponding pair-wave functions[15] are shown in Figs. 4 and 5. For $U=4t$ and $T=0.50t$, an s-wave triplet state has the largest eigenvalue $\lambda_s=0.23$. As seen in Figs. 4(a) and 5(a) (solid circles), the pair-wave function $\phi_s(\mathbf{p},i\omega_n)$ of the s-wave triplet state is even in $\mathbf{p}$ and odd in ω_n. The open circles in Figs. 4(a) and 5(a) represents the pair-wave function $\phi_{s'}(\mathbf{p},i\omega_n)$ which has the second largest eigenvalue $\lambda_{s'}=0.09$. The $d_{x^2-y^2}$-wave singlet state shown as the solid circles in Figs. 4(b) and 5(b) has the third largest eigenvalues $\lambda_d=0.08$. The fourth largest eigenvalue $\lambda_p=0.07$ corresponds to a state that is odd in both ω_n and $\mathbf{p}$, having p_x (or p_y) symmetry [open circles in Figs. 4(b) and 5(b)], hence it is also a singlet.

TABLE I. Monte Carlo results on the largest eigenvalues λ_α of the Bethe-Salpeter equation at different temperatures on an 8×8 lattice for $\langle n\rangle\sim0.87$, and (a) $U=4t$ and (b) $U=8t$. We estimate that the λ values are accurate to $\pm10\%$.

	T/t	λ_s	$\lambda_{s'}$	λ_d	λ_p
(a)	0.50	0.23	0.09	0.08	0.07
	0.25	0.26	0.13	0.17	0.12
(b)	1.0	0.50	0.36	0.05	0.08
	0.50	0.47	0.24	0.15	0.20

As T is lowered from $0.50t$ to $0.25t$, the largest eigenvalue λ_s grows by about 10%, while λ_d more than doubles and λ_p increases substantially. This can be understood in terms of the temperature dependence of $\Gamma_I(p'|p)$. At high temperatures, the irreducible interaction $\Gamma_I(p'|p)$ that enters the Bethe-Salpeter equation is a smooth function of momentum. The pair-wave functions that are smooth in $\mathbf{p}$ but odd in ω_n can make optimum use of the $(\omega_n,\omega_{n'})$ frequency structure of the repulsive

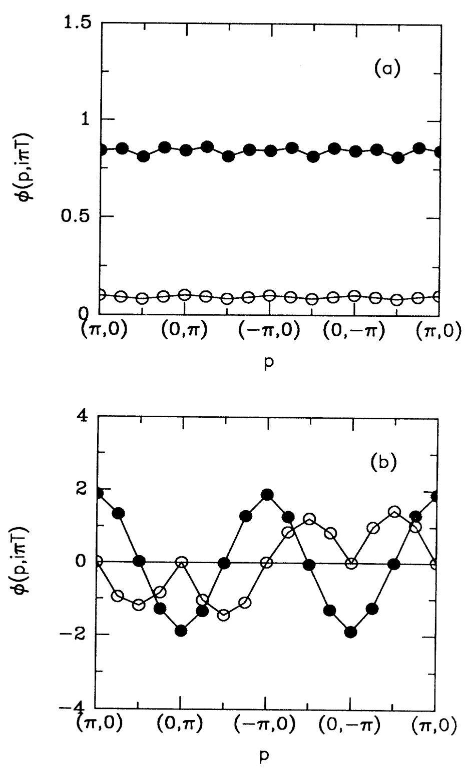

FIG. 4. Monte Carlo results for the gap function $\phi_\alpha(\mathbf{p},i\omega_n)$ vs $\mathbf{p}$ on an 8×8 lattice for $U=4t$, $\langle n\rangle\sim0.87$, and $T=0.50t$. The triplet solutions ϕ_s (solid circles) and $\phi_{s'}$ (open circles) are shown in (a), the singlet solutions ϕ_d (solid circles) and ϕ_{p_y} (open circles) are shown in (b). Here $\omega_n=\pi T$ and $\mathbf{p}$ is taken along the path shown in Fig. 2.

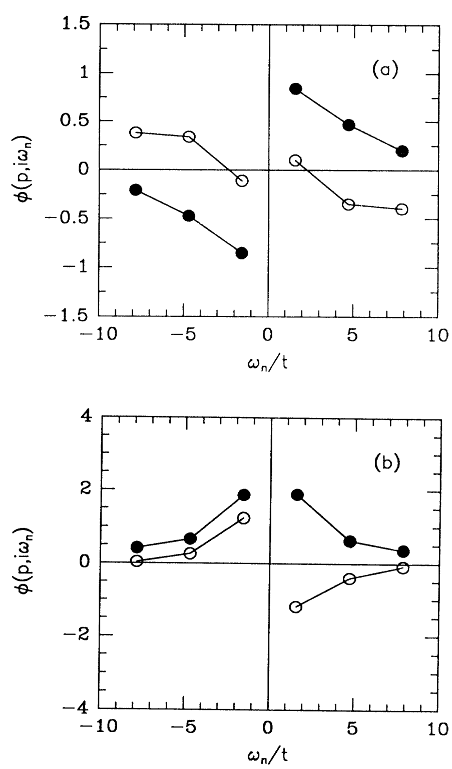

FIG. 5. Monte Carlo results for the gap function $\phi_\alpha(\mathbf{p},i\omega_n)$ vs ω_n on an 8×8 lattice for $U=4t$, $\langle n\rangle\sim0.87$, and $T=0.50t$. The triplet solutions $\phi_s(\mathbf{p},i\omega_n)$ (solid circles) and $\phi_{s'}(\mathbf{p},i\omega_n)$ (open circles) are shown for $\mathbf{p}=(\pi,0)$ in (a). The singlet solutions $\phi_d(\mathbf{p},i\omega_n)$ for $\mathbf{p}=(\pi,0)$ (solid circles) and $\phi_{p_y}(\mathbf{p},i\omega_n)$ for $\mathbf{p}=(\pi/2,\pi/2)$ (open circles) are shown in (b).

$\Gamma_I(p'|p)$ for pairing. However, as the temperature is lowered and $\Gamma_I(p'|p)$ for $\mathbf{p}'-\mathbf{p}=(\pi,\pi)$ grows, the $d_{x^2-y^2}$ and p-wave solutions can make better use of the momentum structure in Γ_I, and their eigenvalues get enhanced. Table I (b) shows the dominant eigenvalues for $U=8t$ at $T=1t$ and $0.5t$. We see that these eigenvalues are larger than those of the $U=4t$ case. It has not been possible to carry out simulations for $U=8t$ at lower temperatures because of the fermion sign problem.

In summary, we have calculated the irreducible particle-particle interaction Γ_I of the Hubbard model using Monte Carlo simulations. We found that as T is lowered, the large momentum transfer structure in $\Gamma_I(p'|p)$ gets enhanced. This is reflected in the solutions of the Bethe-Salpeter equation. Thus at the temperatures for which we have been able to carry out these simulations, the pairing correlations with the largest eigenvalues are associated with an odd-frequency s-wave triplet. However, as the temperature is lowered, we find that the eigenvalues of the $d_{x^2-y^2}$ and p-wave singlet states grow rapidly, suggesting that at low temperatures singlet pairing correlations become dominant.

We thank N. E. Bickers and J. R. Schrieffer for useful discussions. We also thank E. Abrahams, A. Balatsky, and J. R. Schrieffer for sending us a copy of their recent work on odd-ω_n singlet pairing before publication. This work was partially supported by the National Science Foundation under Grant Nos. DMR90-02492 and PHY89-04035. N.B. gratefully acknowledges partial financial support from IBM. S.R.W. would like to thank the Office of Naval Research for support under Grant No. 00014-91-J-1143. This research was also supported in part by the University of California through an allocation of computer time. The numerical calculations reported in this paper were primarily performed at the San Diego Supercomputer Center.

[1]N. E. Bickers, D. J. Scalapino, and R. T. Scaletter, Int. J. Mod. Phys. B **1**, 687 (1987).

[2]N. E. Bickers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **62**, 961 (1989).

[3]P. Monthoux, A. Balatsky, and D. Pines, Phys. Rev. Lett. **67**, 3448 (1991).

[4]J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. B **39**, 11 663 (1989).

[5]G. J. Chen, R. Joynt, F. C. Zhang, and C. Gros, Phys. Rev. B **42**, 2662 (1990).

[6]M. Grilli and G. Kotliar, Phys. Rev. Lett. **64**, 1170 (1990).

[7]S. R. White *et al.*, Phys. Rev. B **40**, 506 (1989); D. J. Scalapino, in *High Temperature Superconductivity,* edited by K. S. Bedell, D. Coffey, D. Meltzer, D. Pines, and J. R. Schrieffer (Addison-Wesley, Reading, MA, 1990), p. 314.

[8]M. Imada and Y. Hatsugai, J. Phys. Soc. Jpn. **58**, 3752 (1989); N. Furukawa and M. Imada, *ibid.* **60**, 3604 (1991).

[9]E. Dagotto and J. R. Schrieffer, Phys. Rev. B **43**, 8705 (1991).

[10]For the parameters and the temperatures we have studied on the 8×8 lattice, the spin-spin correlation length is less than the lattice size so that Γ has essentially reached its bulk behavior.

[11]N. F. Berk and J. R. Schrieffer, Phys. Rev. Lett. **17**, 433 (1966).

[12]In solving the t-matrix and the Bethe-Salpeter equations, Eqs. (3) and (4), we have used an upper frequency cutoff of order the bandwidth.

[13]V. L. Berezinskii, Pisma Zh. Eksp. Teor. Fiz. **20**, 628 (1974) [JETP Lett. **20**, 287 (1974)].

[14]A. Balatsky and E. Abrahams, Phys. Rev. B **45**, 13 125 (1992).

[15]The pair-wave functions are normalized such that $(T/N)\sum_p \phi^2(p)=1$.