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Superconductivity in correlated wave functions

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We describe a new method to numerically evaluate the properties of correlated superconducting wave functions. We have applied it to the resonating-valence-bond (RVB) wave function for the Hubbard model on the square lattice. For the half-filled case we find that the d-wave RVB state and the antiferromagnetic ordered state have the same energy within numerical accuracy. At 10% doping we find d-wave superconductivity, consistent with previous studies. We show that the superconducting order parameter is proportional to the number of holes, for small hole concentrations.

Soon after the discovery of high-T_c superconductivity by Bednorz and Müller,[1] Anderson[2] proposed that the two-dimensional (2D) Hubbard Hamiltonian in the limit of large on-site repulsion U, transformed to an effective Hamiltonian, should be appropriate for modeling these compounds. Recent calculations by Zhang and Rice[3] give additional support to this proposal. Anderson furthermore suggested[2] that a resonating-valence-bond (RVB)-type state may be the ground state, leading to superconductivity (SC) for finite doping and to performed pairs in the half-filled case.

The question whether the 2D Hubbard model has SC ground state is highly controversial. Several mean-field theories have been proposed[4] and indicate various kinds of SC, especially the d and extended (ext) s wave. But the approximations used up to now for the decoupling are not yet under control and therefore the validity of these theories is unclear.

Recently, Lin, Hirsch, and Scalapino[5] exactly diagonalized small systems and Hirsch and Lin[6] and Imada[6] have done quantum Monte Carlo (MC) simulations on finite lattices at quite high temperatures. Their results indicate no tendency towards SC.

In contrast with these results, Gros, Joynt, and Rice[7] examined the two-hole Cooper problem within the Gutzwiller formalism and found a d-wave pairing instability. As an extension of their work, we develop in this paper a new method which makes it possible to evaluate numerically the properties of RVB wave functions for general parameters. The results for the 2D square lattice confirm the qualitative findings of the previous work.[7] Furthermore, these new quantitative results establish the d-wave RVB state as a candidate for the ground state of the antiferromagnetic Heisenberg Hamiltonian in the half-filled case.

Independently, Shiba and Yokoyama[8] have developed a different approach to numerically evaluate RVB wave functions. They use a mixed-band representation for the RVB wave function. Bouchard and Lhuiller[9(a)] have examined, in connection with liquid ^{3}He, a triplet Jastrow-BCS (Bardeen-Cooper-Schrieffer) wave function with equal-spin pairing. They find[9(b)] that for this special case the amplitudes are given by the square root of determinants.

We define the RVB wave function as[2]

$$|\mathrm{RVB}\rangle = \mathrm{const}\times P_{d=0}|\mathrm{BCS}\rangle = \mathrm{const}\times P_{d=0}\prod_{\mathbf{k}}(u_{\mathbf{k}}+v_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle . \quad (1)$$

Here $|\mathrm{BCS}\rangle$ is the usual BCS wave function, with $v_{\mathbf{k}}$ and $u_{\mathbf{k}}$ as variational parameters. $P_{d=0}$ projects on the subspace of no doubly occupied sites and $c^{\dagger}_{\mathbf{k},\sigma}$ are creation operators for fermions. $|0\rangle$ denotes the vacuum. The N-particle component of $|\mathrm{RVB}\rangle$ has the following form:[2]

$$|N\rangle = \mathrm{const}\times P_N|\mathrm{RVB}\rangle = \mathrm{const}\times P_{d=0}\left(\sum_{\mathbf{k}}a(\mathbf{k})c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow}\right)^{N/2}|0\rangle , \quad (2)$$

with $a(\mathbf{k})=v_{\mathbf{k}}/u_{\mathbf{k}}$. P_N projects onto the subspace of N particles. With $a(\mathbf{r})=1/L\sum_{\mathbf{k}}a(\mathbf{k})\exp(i\mathbf{k}\mathbf{r})$, L being the number of lattice sites, $|N\rangle$ takes the following form:

$$|N\rangle = \mathrm{const}\times P_{d=0}\left(\sum_{\mathbf{R}_i,\mathbf{R}'_j}a(\mathbf{R}_i-\mathbf{R}'_j)c^{\dagger}_{\mathbf{R}_i\uparrow}c^{\dagger}_{\mathbf{R}'_j\downarrow}\right)^{N/2}|0\rangle , \quad (3)$$

where $\{\mathbf{R}_i\}$ and $\{\mathbf{R}'_j\}$ denote the positions of the up (down) spins. For singlet (triplet) pairing $a(-\mathbf{r})=\pm a(\mathbf{r})$. Note, that in the half-filled case $|N=L\rangle=|\mathrm{RVB}\rangle$. Furthermore, in the thermodynamic limit, one can work either with $|\mathrm{RVB}\rangle$ or with $|N\rangle$.

The key quantity for a numerical evaluation of (3) is the amplitude of a given spin configuration $\{\mathbf{R}_i\}$, $\{\mathbf{R}'_j\}$. By careful inspection of (3), one can show that this amplitude, apart form a normalization factor, is given by a $N_\sigma\times N_\sigma$ determinant (N_σ is the number of up and down spins, assumed to be equal) with elements $a(\mathbf{R}_i-\mathbf{R}'_j)$. Therefore $|N\rangle$ has the same functional form as the Gutzwiller wave function (GWF), but with different elements in the determinants. For the numerical evaluation of $|N\rangle$ for finite systems, one can then use the same techniques as for the GWF, as described in Refs. 10 and 11. Note that it is possible to work either with fixed particle number or with a fixed phase, since the amplitudes are known for all spin configurations and particle numbers. The results we present in this paper will be mostly for

wave functions with fixed particle number.

Furthermore, this method is not restricted to lattices and the operator $P_{d=0}$. It is straightforward to go to the continuum limit and replace $P_{d=0}$ by a Jastrow weighting factor. Equation (1) becomes then a generalized Jastrow trial wave function for the ground state of superfluid ^{3}He or nuclei (see, e.g., Ref. 9).

In the limit of large on site repulsion U, the Hubbard Hamiltonian transforms[12] into the following effective Hamiltonian, valid in the subspace of no doubly occupied sites ($n=N/L\leq 1$):

$$H_{\rm eff}=T+H_{\rm eff}^{(2)}+H_{\rm eff}^{(3)},\quad T=-t\sum_{\langle i,j\rangle,\sigma}a_{i,\sigma}^{\dagger}a_{j,\sigma}+\text{H.c.},$$
$$H_{\rm eff}^{(2)}=4t^2/U\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-n_in_n/4), \tag{4}$$
$$H_{\rm eff}^{(3)}=-t^2/U\sum_{i,\tau\neq\tau',\sigma}(a_{i+\tau,\sigma}^{\dagger}a_{i,-\sigma}^{\dagger}a_{i,-\sigma}a_{i+\tau',\sigma}+a_{i+\tau,-\sigma}^{\dagger}a_{i,\sigma}^{\dagger}a_{i,-\sigma}a_{i+\tau',\sigma}).$$

Here $\mathbf{S}_i$ are the spin operators on site i, $a_{i,\sigma}^{\dagger}=(1-n_{i,-\sigma})c_{i,\sigma}^{\dagger}$ with $n_i=n_{i,\downarrow}+n_{i,\uparrow}$, $n_{i,\sigma}=c_{i,\sigma}^{\dagger}c_{i,\sigma}$. $\langle i,j\rangle$ are pairs of nearest-neighbor (NN) sites and $i+\tau$ denotes a NN site of i. T is the kinetic energy of the holes and $H_{\rm eff}^{(2,3)}$ the two- and three-site contributions, respectively. In the half-filled case, $H_{\rm eff}$ reduces to the antiferromagnetic Heisenberg Hamiltonian.

To examine the ground state, we have investigated a set of trial wave functions of the form of (2). The normal state is the GWF and has $a(\xi_{\mathbf{k}}<0)=1$, $a(\xi_{\mathbf{k}}>0)=0$, with $\xi_{\mathbf{k}}=-2t[\cos(k_x)+\cos(k_y)]-\mu$. Here μ is the chemical potential. For the SC state we used the standard BCS parametrization:

$$a(\mathbf{k})=\Delta(\mathbf{k})/[\xi_{\mathbf{k}}+\sqrt{\xi_{\mathbf{k}}^2+\Delta^2(\mathbf{k})}]$$

with

$$\Delta(\mathbf{k})\equiv\Delta\ (s\text{ wave}),$$
$$\Delta(\mathbf{k})=\Delta[\cos(k_x)-\cos(k_y)]\ (d\text{ wave}), \tag{5}$$
$$\Delta(\mathbf{k})=\Delta[\cos(k_x)+\cos(k_y)]-\mu\ (\text{ext } s\text{ wave}).$$

Note that Δ is a variation parameter and not the order parameter. The true SC order parameter vanishes like $1-n$, as $n\rightarrow 1$, as will be discussed below.

For the half-filled case, the extended s wave is identical with the GWF, since then $\Delta(\mathbf{k})\sim\xi_{\mathbf{k}}$ and the two functions $a(\mathbf{k})$ are equivalent by means of a linear transformation. Similar arguments can be used to show that the d wave for $n=1$ approaches asymptotically the GWF as $\Delta\rightarrow\infty$.

We discuss first the results for the half-filled case. We find that the s wave has its energy minimum at $\Delta=0$ which is[13] $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle_{\Delta=0}=-0.267\pm0.003$. The d wave gains about 20% with respect to the value at $\Delta=0$. It has a broad minimum between $0.3t<\Delta<3.0t$. $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$ is practically size independent. For $\Delta=t$ its value is -0.319 ± 0.01 [see Fig. 1(a)]. For the antiferromagnetically ordered Gutzwiller state Yokoyama and Shiba[13] obtained -0.321 ± 0.001. By diagonalization of small systems and extrapolation to the thermodynamic limit, Oitmaa and Betts[14] estimated for the ground state of the antiferromagnetic Heisenberg Hamiltonian -0.328 ± 0.003, within the numerical accuracy of our result. We therefore conclude that further numerical work is required to definitively establish the nature of the ground state of the model.

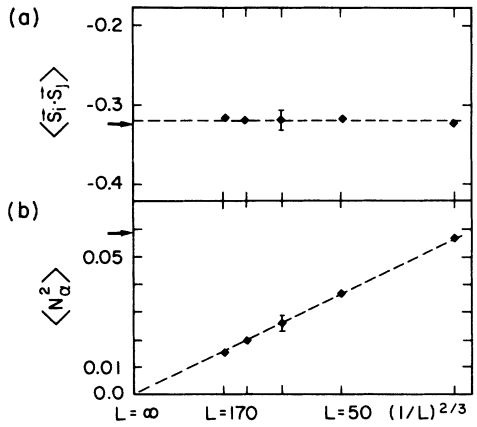

FIG. 1. Data for the half-filled case ($n=1$) and the d-wave RVB state with $\Delta=t$. The NN spin-spin correlation (a) and the squared staggered magnetization (b) are plotted as a function of $(1/L)^{2/3}$ for lattices with a total number of sites $L=26$, 50, 82, 122, 170. Typical error bars are shown. The arrows indicate the estimates of Oitmaa and Betts (Ref. 14) for the ground state of the 2D antiferromagnetic Heisenberg Hamiltonian. Between 7×10^3 and 7×10^4 MC steps per site have been used.

We have examined the size dependence the staggered magnetization[14] squared $\langle N_a^2\rangle=\langle(1/L\sum_i\epsilon_iS_i^z)^2\rangle$ and found that it scales with $(1/L)^{2/3}$. Figure 1(b) shows that $\langle N_a^2\rangle$ extrapolates to zero in the thermodynamic limit. We conclude therefore that this RVB state has no long-range magnetic order.

We also did calculations for $n\sim0.9$, $L=82$, and $N_h=L-N=8$ holes. The results for the s and d waves are shown in Fig. 2. We show all contributions to $\langle H_{\rm eff}\rangle$ separately in units appropiate to their physical significance. We do not show the results for the extended s waves, which lie in between that of the s and the d waves. In particular, we find no energy gain for $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$ or for $\langle H_{\rm eff}\rangle$ for the extended s wave.

We choose a reasonable value, for the high-T_c compounds, of $U/t=16$, to show that for the d wave, the gain in $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$ [Fig. 2(c)] is enough to overcome the loss in kinetic energy [Fig. 2(b)]. The total energy [Fig. 2(a)] shows a clear minimum at $\Delta\sim0.55t$. To show that this is the case, despite the large error bars of Fig. 2(a), we have calculated for $\Delta=0$, $\Delta=0.55t$, and d-wave pairing, $\langle H_{\rm eff}\rangle$ with higher accuracy. The results $\langle H_{\rm eff}\rangle_{\Delta=0}=-0.484\pm0.002t$ and $\langle H_{\rm eff}\rangle_{\Delta=0.55t}=-0.494\pm0.006t$ show clearly that the energy minimum is at finite Δ.

In Fig. 2(e) we see that the s wave gains from the three-site contributions, but this gain does not compensate the loss in kinetic energy [Fig. 2(b)] since $\langle H_{\rm eff}^{(3)}\rangle\sim(1-n)t^2/U$ and is therefore one order of magnitude smaller than $\langle T\rangle\sim(1-n)t$.

In Fig. 2(d) the NN hole-hole correlation is plotted.

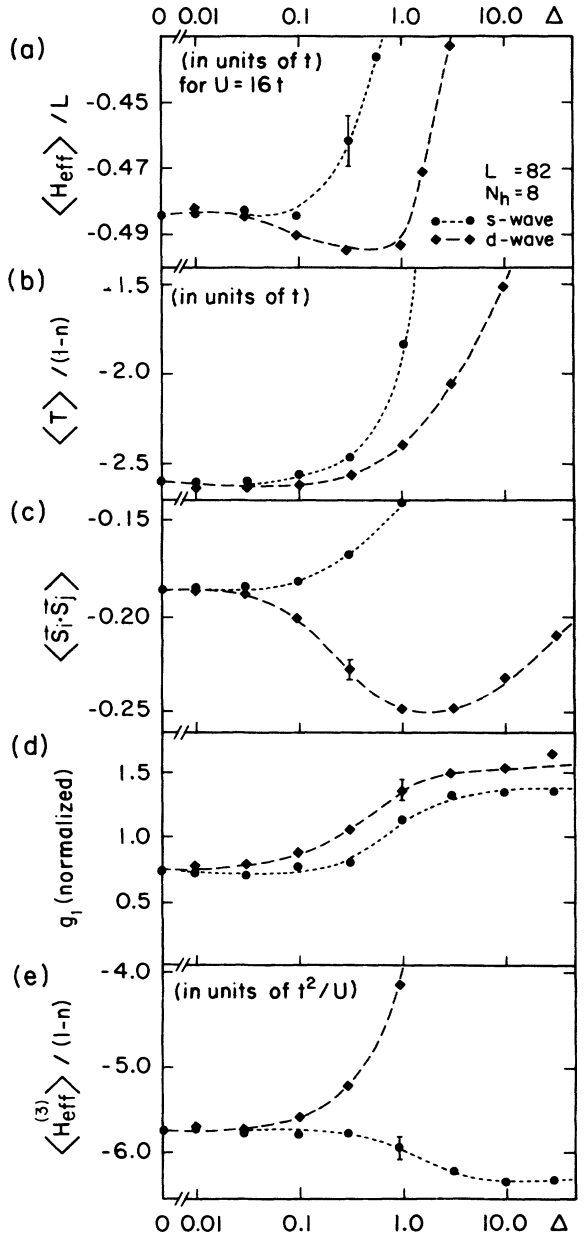

FIG. 2. Data for $L=82$ sites and $N_h=8$ holes, for the d wave (squares) and the s waves (circles), as a function of Δ in units of t. Typical error bars are shown, all points have been calculated with the same accuracy. In (a) the total energy per site for $U=16t$ is shown, in (b) the kinetic energy per hole, in (c) the NN spin-spin correlation, in (d) the NN hole-hole correlation $g_1=(1-n)^{-2}\langle(1-n_{i,\downarrow})(1-n_{i,\uparrow})(1-n_{j,\downarrow})(1-n_{j,\uparrow})\rangle$, and in (e) the three-site contribution per hole. Note that the d wave gains about 35% in $\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle$ for $\Delta\sim t$. About 3×10^3 MC steps per site have been used.

Consistent with previous findings[7] at the optimal value of $\Delta\sim0.55t$, it is not greatly enhanced for this lattice size with respect to $\Delta=0$.

We now discuss the SC order parameter, as defined in the recent mean-field calculations:[4] $\Delta_1=1/L\sum_i \times\langle c^\dagger_{i,\sigma}c^\dagger_{i+\tau,-\sigma}\rangle$ where i, $i+\tau$ are NN sites. The generalized Gutzwiller approximation[11] yields

$$\Delta_1^{\mathrm{RVB}}=(1-n)\Delta_1^{\mathrm{BCS}}/(1-n/2)\,. \tag{6}$$

To show that (6) holds for small $1-n$ we have calculated

$$\Delta_{\mathrm{eff}}=\langle L\,|\,c^\dagger_{i,\sigma}c^\dagger_{j,-\sigma}\,|\,L-2\rangle/\sqrt{\langle L-2\,|\,L-2\rangle\langle L\,|\,L\rangle}$$

for wave functions with, on the average, one hole (i.e., $1-n=1/L$). In Table I the x component of $(1-n/2)/(1-n)\Delta_{\mathrm{eff}}$ is given for d-wave pairing. The y component has the opposite sign. Also shown (in parentheses) are the corresponding BCS values. We see that Eq. (6) is qualitatively well fulfilled for a wide range of Δ and hole densities. Therefore Δ_1 is truly a SC order parameter, since it vanishes for a Fermi liquid, which is a incoherent superposition of states with different particle numbers, in a grand canonical ensemble.

TABLE I. The x component of the SC order-parameter for d-wave pairing. Shown are the values for $(1-n/2)/(1-n)\times\langle c^\dagger_{i,\sigma}c^\dagger_{j,-\sigma}\rangle_{\mathrm{RVB}}$ and the statistical errors. $\langle c^\dagger_{i,\sigma}c^\dagger_{j,-\sigma}\rangle_{\mathrm{BCS}}$ are given with parentheses. The wave functions have, on the average, one hole on L sites [i.e., $(1-n)=1/L$]. Δ is in units of t.

L \ Δ	0.1	0.3	1.0
16			0.179 ±0.029 (0.139)
36			0.186 ±0.031 (0.144)
64	0.101 ±0.040 (0.058)	0.162 ±0.041 (0.097)	0.181 ±0.025 (0.146)

In summary, we have developed a new algorithm to evaluate numerically RVB and generalized Jastrow wave functions. It is very fast and not restricted to a special choice of parameters. We applied this algorithm to the RVB wave function on the 2D square lattice. Our result support Anderson's suggestion[2] that even for the half-filled case an RVB-type wave function might be the ground state or very close in energy to the ground state, since we find that the energy for a d-wave RVB wave function agrees within numerical accuracy with the other estimates for the ground-state energy of the 2D antiferromagnetic Heisenberg model. We also showed that this RVB state has no magnetic long-range order in the thermodynamic limit. For finite doping we find d-wave superconductivity in agreement with previous results.[7] We have shown that the superconducting order parameter is proportional to $1-n$ as n approaches 1.

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