PHYSICAL REVIEW B VOLUME 47, NUMBER 17 1 MAY 1993-I

New phase in the one-dimensional t-J model

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(Received 7 December 1992)

A new phase of a gas of pairs of electrons bounded in a singlet state is found in the one-dimensional t-J model for $J > 2t$ and the density of electrons less than 0.2. This phase was conjectured in the study of the diagonalization of small lattices [Phys. Rev. Lett. **66**, 2388 (1991)]. The existence of this new phase for much larger lattice sizes is demonstrated by a combination of two numerical methods, the variational Monte Carlo and the power method. A trial wave function for this phase is proposed and shown to be in good agreement with the ground state obtained by the power method.

Recently there is a great interest in understanding the t-J model in one dimension. It is believed that the knowledge gained will become very useful in the pursuit of solving the t-J model in two dimensions which has been widely accepted as the model for high-temperature superconductors. The non-Fermi-liquid behavior of the one-dimensional t-J model could very well lay the basis for understanding high-temperature superconductors as emphasized by Anderson.[1]

The phase diagram of the one-dimensional t-J model was studied by Ogata *et al.*[2] using the method of exact diagonalization. It shows that there are two phases, the Lüttinger liquid without a spin gap and the particle-hole separated phase when the magnetic interaction J is much larger than the charge hopping energy t. When J gets larger than $2t$, the superconducting correlation becomes dominant in the Lüttinger liquid. It was mentioned that in the low-density region there may be a phase with two particles bounded. Because of the limit in using small lattice sizes it has not been able to provide conclusive results about this phase.

On the other hand variational methods have been quite useful to obtain some ideas about the phase diagram and ground-state properties for larger lattice sizes. Recently Hellberg and Mele[3] (HM) have proposed a variational wave function that successfully reproduces the phase diagram obtained from the exact diagonalization[2] but with some differences. In the low-density region, HM wave function seems to imply the existence of a third phase.

To determine the phase diagram from a variational study is obviously quite risky. For instance, it is not known how close to the ground state is the optimized trial wave function with the lowest variational energy. The choice of wave function pretty much determines the possible phases. Hence it is important to find a method to provide some guidance about the validity of the variational results.

In this paper we use a method that systematically improves the variational wave function and provides information about its relation to the ground state. In fact it may also produce the ground state. This method known as the power method[4] projects out the ground state from a trial wave function by applying large powers of the Hamiltonian.

Below we shall first briefly discuss the numerical procedures of the power method. In most regions of parameter space HM wave function is a very good approximation to the exact ground state.[4] But for $J > 2t$ and in the low-density region, comparing to the ground-state superconducting pairing correlation is substantially underestimated by HM. To better represent the ground state we propose a wave function of singlet pairs of bounded electrons. This state is then shown to agree with the ground state obtained by the power method. This state has a spin excitation gap. At the end we shall briefly mention the possibility of bounded states with more than two particles.

The Hamiltonian of the one-dimensional t-J model written in the subspace of no doubly occupied sites has two terms,

$$H_t = -t \sum_{i\sigma} C^{\dagger}_{i\sigma} C_{i+1\sigma} + \text{H.c.} \tag{1}$$

and

$$H_J = J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \tfrac{1}{4} n_i n_{i+1}) \ . \tag{2}$$

This model has been solved exactly at[5] $J=0$ and[6] $J=2t$ by using the Bethe ansatz solutions. In both of these cases, the ground states belong to an unconventional class of interacting Fermi systems known as the Lüttinger liquid;[7] which exhibit power-law singularities in correlation functions and the momentum distribution at the Fermi surface.[8]

It is possible to obtain the ground-state wave function by using a projection method. Given a trial wave function $|\psi\rangle$ that is not orthogonal to the ground state of a Hamiltonian H, applying the operator $(W-H)^p$ to $|\psi\rangle$ will project out the ground state as the power p approaches infinity. The constant W is chosen such that all the excited states with energy E_i satisfies the relation $|(W-E_i)/(W-E_g)| < 1$ where E_g is the ground-state

energy. For the t-J model we may choose $W=0$.

This method has been used in the spin systems by many authors.[9-12] It is a simplified version of the Green's function Monte Carlo method.[13,14] Details of our approach can be found in Ref. 4.

To calculate the expectation value of an operator O in the ground state we need to calculate the two quantities $\langle p|O|p\rangle$ and $\langle p|p\rangle$, where $|p\rangle=(-H)^p|\psi\rangle$ and $|\psi\rangle$ is the trial wave function. The numerical technique we shall use is a combination of the variational Monte Carlo (VMC) method and the Neumann-Ulam matrix method.[15] First, the trial wave function is expanded in a complete orthonormal set, $|\psi\rangle=\sum_\alpha a_\alpha|\alpha\rangle$. We then have

$$\langle p|p\rangle=\sum_\alpha |a_\alpha|^2 M(\alpha)\ , \tag{3}$$

where

$$M(\alpha)=\sum_\beta a_\beta^*/a_\alpha^*\langle\beta|H^{2p}|\alpha\rangle\ . \tag{4}$$

After the configuration $|\alpha\rangle$ is chosen with the probability

$$Pr(\alpha)=|a_\alpha|^2/\sum_\gamma |a_\gamma|^2 \tag{5}$$

by using the Metroplis method, we are left to calculate $M(\alpha)$ of Eq. (4). This is equivalent to evaluating the matrix element $(H^{2p})_{\alpha\beta}$. Each matrix element $(-H)_{\alpha\beta}$ is decomposed into the product of a transition probability and a residual weight[14,15] as

$$(-H)_{\alpha\beta}=P_{\alpha\beta}w_{\alpha\beta} \tag{6}$$

with

$$\sum_\beta P_{\alpha\beta}=1 \quad \text{and} \quad P_{\alpha\beta}\geq 0\ . \tag{7}$$

For simplicity we have chosen $w_{\alpha\beta}=w_\alpha=\sum_\beta(-H)_{\alpha\beta}$. $M(\alpha)$ is evaluated by generating many random walk paths with length $2p$ and each step is chosen by the probability $P_{\alpha\beta}$. The score of a path from $\alpha\to\alpha_1\to\alpha_2\to\cdots\to\beta$ is given by $w_{\alpha\alpha_1}w_{\alpha_1,\alpha_2}\cdots w_{\alpha_{2p-1},\beta}(a_\beta^*/a_\alpha^*)$. The mean value of the score is exactly $M(\alpha)$.

In principle the ground state almost always can be projected out no matter what the choice of the trial wave function $|\psi\rangle$ is. But in practice a good trial wave function is essential to ensure fast convergence without using very large powers for larger lattices. The wave function proposed by Hellberg and Mele[3] ($|\mathrm{HM}\rangle$) was shown in Ref. 4 to be a very good trial function. $|\mathrm{HM}\rangle$ is a product of the spin and hole wave functions with the constraint that each site of the lattice is allowed to have at most one particle. The spin wave function is just the ideal Fermi-gas wave function. The coefficient a_α^S is a product of two determinants $\det[\phi_k(r_i^\uparrow)]\ \det[\phi_k(r_j^\downarrow)]$, where $\phi_k(r_i)=\exp(ikr_i)$. The determinant is proportional to the Vandermonde determinant when the values of k are chosen as $k=-k_F+l\Delta k$, $l=0,1,\ldots,N_\sigma-1$ where N_σ is the number of electrons with same spin. Hence for a spin configuration $|\alpha\rangle$ the coefficient is of the form

$$a_\alpha^S=\prod_{i<j}\sin[\Delta k(r_i^\uparrow-r_j^\uparrow)/2]\prod_{l<m}\sin[\Delta k(r_l^\downarrow-r_m^\downarrow)/2]\ . \tag{8}$$

The hole wave function involving long-range correlations has the coefficient $\Pi_{i<j}|\sin[\Delta k(r_i^0-r_j^0)/2]|^\nu$, where r^0 denotes the positions of the holes. The holes repel each other when ν is positive and attract otherwise. For $\nu=0$ the state $|\mathrm{HM}\rangle$ simply becomes the famous Gutzwiller wave function $|\mathrm{GW}\rangle$.[16]

We have found[4] that applying the power $(-H)^p$ to the $|\mathrm{HM}\rangle$ hardly changes the values of the energy, the spin structure factor, the charge structure factor, the momentum distribution, and the pairing correlation for most values of t/J and particle density. In other words $|\mathrm{HM}\rangle$ is very close to the ground state such that the variational result ($p=0$) is almost the same as the results with very large power p. Only in a region of low-particle density, n_e less than 0.2, we found substantial increase of the pairing correlation as power p increases.

The pairing correlation function is defined as

$$P(k)=\frac{1}{L}\sum_{i,j} e^{ik(r_i-r_j)}\langle\Delta^\dagger(i)\Delta(j)\rangle\ , \tag{9}$$

where the pairing operator $\Delta(i)=C_{i\uparrow}C_{i+1\downarrow}-C_{i\downarrow}C_{i+1\downarrow}$. In Fig. 1 the value of $P(k=0)$ is plotted as a function of the power for $J=3t$. The trial wave function is $\nu=-0.5$ HM state. The particle density is $n_e=\frac{1}{6}$ for three lattice sizes, $L=12$ (squares), $L=24$ (triangles), and $L=36$ (circles). The value of $P(k=0)$ is much larger for the ground state than what $|\mathrm{HM}\rangle$ represents. The larger the lattice the larger the difference is. Clearly a better wave function is needed to understand the ground state.

When there are only two electrons in an infinite chain, the ground state is easily found. For $J>2t$, the pair forms a singlet bound state. Its wave function is of the form $\sum_{n=1}^\infty(2t/J)^{n-1}b_n^\dagger|0\rangle$, where the operator $b_n^\dagger=\sum_i C_{i\uparrow}^\dagger C_{i+n\downarrow}^\dagger-C_{i\downarrow}^\dagger C_{i+n\uparrow}^\dagger$, and the ground-state ener-

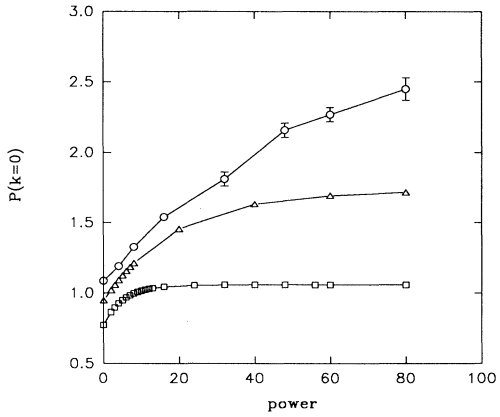

FIG. 1. The pairing correlation $P(k=0)$ as a function of power for $J=3t$. There are three lattice sizes: $L=12$ (squares), $L=24$ (triangles), and $L=36$ (circles) for the same particle density $n_e=\frac{1}{6}$. $\nu=-0.5$ HM state is used as the trial wave function.

gy is $\epsilon_0 = -J - 4t^2/J$. The size of the pair is approximately $1/\ln(J/2t)$. For $J/t = 2.5-3.5$ the size of pair is sufficiently small that we can have many pairs in the lattice without having substantial overlap between them.

Hence we propose the following wave function for a gas of single pairs (SP):

$$|\mathrm{SP}\rangle = Pd\left[\sum_{n=1}^{\infty}\left[\frac{2t}{J}\right]^{n-1} b_n^{\dagger}\right]^{N_e/2}|0\rangle\ , \tag{10}$$

where N_e is the total number of particles and Pd is the projection operator that forbids two particles occupying the same site. This wave function is of a particular form of the projected BCS state or the RVB state.[17]

The variational energy of $|\mathrm{SP}\rangle$ is compared with that of $|\mathrm{HM}\rangle$ for different ν. Notice that SP wave function has no variational parameters. The phase diagram based on this variational calculation is shown in Fig. 2. The dashed line is the original phase diagram of HM[3] and the solid line shows the new singlet phase.

As long as the density of particles n_e is low enough such that there is no sufficient overlap between pairs, the energy per particle is just half the energy of a bounded pair, $\epsilon_0/2$. Hence for an ideal gas of singlet pairs the variational energy per site for $|\mathrm{SP}\rangle$ is just $E_{\mathrm{SP}} = -(n_e/2)(J + 4t^2/J)$. The energy of a phase separated state[2] is $-n_e J \ln 2$. Thus for $J > 3.218t$ the gas of singlet pairs will condense. It is expected to be a first-order transition between the SP phase and the phase-separated state. When the particle density is substantial, the pairs overlap and interact strongly it becomes less meaningful to discuss the ground state in terms of pairs. In this situation HM wave function includes correlation between all particles and is expected to have a better variational energy.

The phase diagram of Fig. 2 only suggests the possible existence of the new singlet pair phase. To verify it we apply the power method and examine energy and various correlation functions as a function of power. In Fig. 3 energy per site as a function of power is plotted for $J = 3t$ with both HM and SP variational states. There are 6 particles in 60 sites, i.e., $n_e = \frac{6}{60}$. While energy of HM (empty circles) has decreased more than 1% with increasing power, the energy of SP (solid circles) hardly varies and it has the limiting value given by E_{SP}.

In Fig. 4 the static spin structure factor is plotted as a function of wave vector k for $J = 3t$ and $n_e = \frac{6}{60}$. The solid circles are the results of SP without power and it cannot be differentiated from the result of power $= 20$. The solid line is the expected result of an ideal gas of singlet pairs:

$$S(k) = \left[\frac{n_e}{4}\right][1 - \cos(ka)] \times \frac{1 + (2t/J)^2}{1 + (2t/J)^4 - 2(2t/J)^2\cos(ka)}\ . \tag{11}$$

The triangles in Fig. 4 are the results of $\nu = -0.5$ HM state for power $= 0$, the empty circles are for power $= 10$, and the squares for power $= 20$. The result of HM has not yet converged for power $= 20$, but it clearly approaches the SP result as the power increases.

It is easy to show that[18] the structure factor $S(k)$ would be proportional to k^2 for small k if there is a spin excitation gap. Quite clearly HM wave function represents the Lüttinger liquid without a spin gap, its $S(k)$ varies linearly with k. Whereas the SP state as shown in Eq. (11) varies with k^2. Since the results of SP state hardly changes with the power, we believe that the ground state indeed has a spin gap.

The particle-particle correlation or the charge structure factor has also been studied and is found to be peaked near very small wave vector k for both SP and HM wave functions. The results are consistent with a ground state without a charge gap.

The pairing correlation function, $P(k)$ of Eq. (9), for the SP state has a δ-function-like peak at $k = 0$. This is

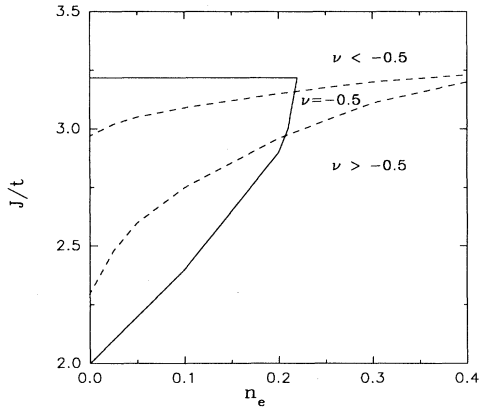

FIG. 2. The phase diagram of the t-J model determined by HM and SP variational wave functions. The dashed lines are the results obtained by Hellberg and Mele (Ref. 3). The phase-separated state is marked by $\nu < -0.5$. The solid line encloses the region where the singlet pair state of Eq. (10) has lower variational energy than the HM state.

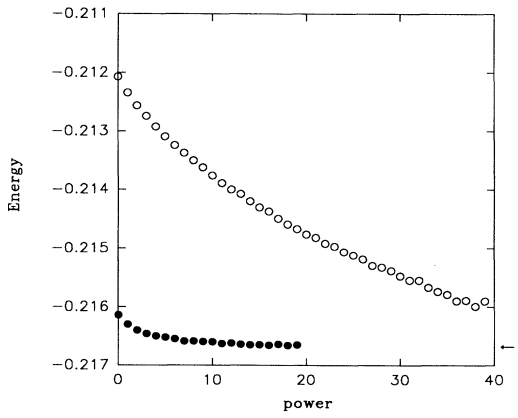

FIG. 3. Energy per site as a function of power for $J = 3t$ and particle density $n_e = \frac{6}{60}$. The empty and solid circles are the results of using $\nu = -0.5$ HM state and SP state, respectively. The arrow indicates the energy E_{SP} discussed below Eq. (10).

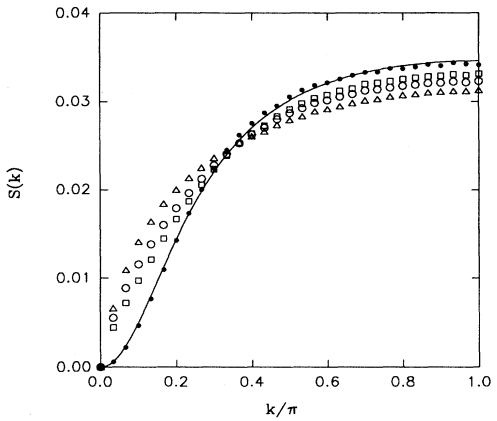

FIG. 4. The spin structure factor, $S(k)$, as a function of the wave vector k for a lattice of 6 holes in 60 sites and for $J=3t$. The solid circles are the variational results of the SP state. The solid line is the result of ideal gas of singlet pairs given by Eq. (11). The triangles, empty circles, and squares are the results of power =0, 10, and 20, respectively, using the HM trial wave function.

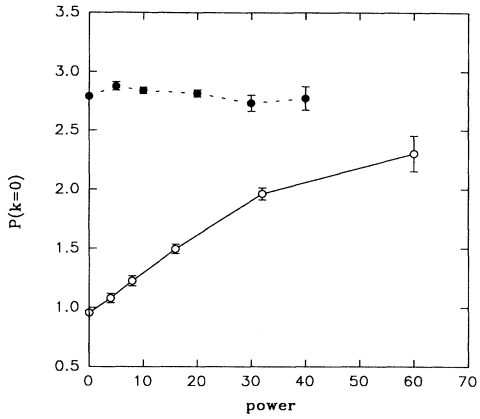

FIG. 5. The pairing correlation function $P(k=0)$ as a function of power for $J=3t$ and $n_e=\frac{6}{60}$. The empty and solid circles are the results of using $\nu=-0.5$ HM state and SP state, respectively.

very different from the Lüttinger-liquid[4,7] behavior where $P(k)\sim k^{1/K_Q}$ for small k. In Fig. 5 $P(k=0)$ is plotted as a function of power for $J=3t$ and $n_e=\frac{6}{60}$. The value of $P(k=0)$ for HM state is more than doubled while the value for SP is unchanged within the statistical errors.

In conclusion, we have shown that there is possibly a new phase of a gas of singlet pairs for the one-dimensional t-J model. A trial wave function for this phase is proposed. Using the power method that projects out the ground state from a variational state, we find that the energy, the spin correlation, and the pairing correlation of this new trial function are almost identical with the projected ground state. The very successful wave function proposed by Hellberg and Mele[3] does not fare so well in this region.

So far we have avoided the discussion of interaction between these pairs. It is self-evident that there is attractive interaction between the pairs so a phase-separated state can be formed. This effect can also be seen from Fig. 3. The wave function of Eq. (10) implicitly introduces a repulsion between the pairs by obeying the Pauli statistics and imposing the constraint of no two particles occupying the same site. Hence the variational energy is always higher than the ideal noninteracting gas of pairs. The ground-state energy obtained by the power method seems to agree with this ideal value very well. The Hamiltonian has an effective attractive interaction between pairs to balance out the repulsion due to statistics and the projection operator. We have also found the ground-state energy to be lower than the energies of both the ideal SP and the phase-separated states near their phase boundary. It is suggestive that states with more than two particles bounded may exist in the low-density region. The boundary of the phase-separated state may be pushed to even larger values of J/t.

The authors are grateful to the hospitality of the Material Science Center and Department of Physics of National Tsing Hua University, where most of the numerical work reported in this paper were carried out. This work was partially supported by the National Science Council of Republic of China, Grant No. NSC81-0511-M007-509.

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