PHYSICAL REVIEW B VOLUME 44, NUMBER 3 15 JULY 1991-I

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Composite-fermion theory for the strongly correlated Hubbard model

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(Received 26 December 1990)

We study a class of variational wave functions for strongly correlated systems by expanding the electron operators as composites of spin-$\frac{1}{2}$ Fermi fields and spinless Fermi fields. The composite particles automatically satisfy the local constraint of no double occupancy and include correlations between opposite-spin particles in a very physical way. We calculate the energy and correlation functions for the one-dimensional $U=\infty$ Hubbard model, where a comparison with exact results is made. The method is computationally very tractable and can readily be generalized to higher dimensions.

Recent interest in the Hubbard Hamiltonian in the strongly correlated ($U \gg t$) limit has stimulated development of a number of schemes for describing the low-energy spectrum in this model.[1-6] In this paper we discuss a variational approach for this problem which is quite successful at describing the energy and two-point correlation functions of the infinite U model in one dimension, for which the exact solution is available for comparison.[7] We briefly outline our computational approach and compare results from our wave functions with the exact solution and with results from the Gutzwiller wave function. The method can easily be applied in higher dimensions and to systems with intersite interactions, such as the t-J model.

The Hubbard Hamiltonian is written as

$$H=-t\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where $\langle ij\rangle$ is the sum over nearest-neighbor pairs. We consider here the $U=\infty$ limit where double occupation of a single site by an up and down electron is forbidden.

Our construction is motivated by the observation that the Gutzwiller wave function (GW), which is perhaps the simplest constrained many-fermion state one can construct for this problem, already provides a many-body state with a very competitive kinetic energy. The GW is obtained by a projection of a noninteracting Fermi sea onto the subspace with no doubly occupied sites, in the manner,

$$|\Psi_G\rangle=P_d|\Psi_0\rangle \tag{2}$$

where

$$P_d=\prod_i(1-n_{i\uparrow}n_{i\downarrow}),\ \ |\Psi_0\rangle=\prod_{|k|<k_F}c_{k\uparrow}^{\dagger}c_{k\downarrow}^{\dagger}|0\rangle\,.$$

The optimization of the single-particle kinetic energy before projection tends to provide a correlated many-body state with a very low kinetic energy. This procedure is widely used, and has enjoyed a number of noteworthy successes.[1-3]

However, the GW is plagued by several well-known pathologies. Even in one dimension, the one-particle momentum distribution in the GW exhibits a single discontinuity on a Luttinger Fermi surface at k_F. This feature disagrees with the known behavior of the Bethe ansatz solution in one dimension which shows power-law singularities in $n(k)$ at both k_F and $3k_F$.[8-10] (The analogous behavior of the two-dimensional model is interesting and controversial.) Additionally, the GW tremendously underestimates the spin correlations in the ground state. These failures are not surprising and originate, in part, from the unphysically sharp correlation hole introduced between opposite-spin particles in the GW.

In this paper we study a class of variational wave functions for the strongly correlated Hubbard model which retain a number of desirable properties of the GW while eliminating several of its difficulties in a controlled and physical way. Indeed, exactly at half filling, our approach is equivalent to a strict Gutzwiller projection, while away from half filling our theory provides a significant improvement of both the kinetic energy and correlation functions relative to the GW.

To construct our wave functions, we expand the single-electron operators in terms of composite fermions and examine two mean-field decompositions of the composite operators. We set the single electron creation operator equal to a product of three fermion creation operators, each acting on a different "species" of fermion, which we write as $c_{i\sigma}^{\dagger}=s_{i\sigma}^{\dagger}f_i^{\dagger}g_i^{\dagger}$. The $s_{i\sigma}^{\dagger}$ operate on a spin-$\frac{1}{2}$ fermionic field, while $f_i^{\dagger}$ and $g_i^{\dagger}$ are spinless Fermi operators. The motion of the physical electrons forces all three species of the product particle to move in unison. Thus the Fermi nature of the spinless fields forbids double occupancy of any site, while the product of three Fermi fields ensures that the composite operator $c_{i\sigma}^{\dagger}$ retains the correct "constrained" Fermi statistics.[11]

This procedure will be recognized as a generalization of the frequently employed slave boson approach for strongly correlated electrons,[4,5] and amounts to replacing the slave boson operator by a factorization in terms of a product of the fermion fields $f^{\dagger}$ and $g^{\dagger}$. This latter step has the important consequence of enforcing the hard-core constraint in the dynamics of the auxiliary product field $f^{\dagger}g^{\dagger}$ and can avoid an unphysical condensation of the auxiliary field.

We write the $U=\infty$ Hubbard Hamiltonian (1) in terms of the composite fields as

$$H_{\text{comp}}=-t\sum_{\langle ij\rangle\sigma}(s_{i\sigma}^{\dagger}f_i^{\dagger}g_i^{\dagger}g_jf_js_{j\sigma}+\text{H.c.}) \tag{3}$$

with the local constraint $s_{i\sigma}^{\dagger}s_{i\sigma}=f_i^{\dagger}f_i=g_i^{\dagger}g_i$ to ensure occupation of a given site by either no fermions or three fermions, one from each species. We note that the Hamiltonian is invariant under the following gauge transformations:

$$s_{i\sigma}^{\dagger}\rightarrow e^{i\theta_i}s_{i\sigma}^{\dagger}\,,\quad f_i^{\dagger}\rightarrow e^{-i\theta_i}f_i^{\dagger}\,,$$

$$s_{i\sigma}^{\dagger}\rightarrow e^{i\phi_i}s_{i\sigma}^{\dagger}\,,\quad g_i^{\dagger}\rightarrow e^{-i\phi_i}g_i^{\dagger}\,.$$

An integral over the local parameters θ_i and ϕ_i exactly enforces the required constraint on the number densities.

To generate our first trial wave function we employ a standard mean-field decoupling of each species of fermion and rewrite the Hamiltonian (3) as

$$H_f^{\text{MF}}=-t\sum_{\langle ij\rangle\sigma}[\langle s_{i\sigma}^{\dagger}s_{j\sigma}\rangle\langle f_i^{\dagger}f_j\rangle\langle g_i^{\dagger}g_j\rangle+\text{H.c.}]\,. \tag{4}$$

We write the ground state of the auxiliary fermion Hamiltonian as a product of determinantal wave functions of single-particle states for each field with identical particle coordinates:

$$\Psi_f=F(r_j^{\uparrow},r_j^{\downarrow})\;G(r_j^{\uparrow},r_j^{\downarrow})\;S(r_j^{\uparrow},r_j^{\downarrow}) \tag{5}$$

where $F=G=\text{Det}[\phi_{k_i}(r_j^{\uparrow},r_j^{\downarrow})]$ and $S=\text{Det}[\phi_{k_i}(r_j^{\uparrow})]\times\text{Det}[\phi_{k_i}(r_j^{\downarrow})]$. The F and G are determinants of *all* particle coordinates, while S is the product of determinants for each spin. We consider only the subspace with equal numbers of up and down electrons and choose the single-particle basis states to be plane waves, so a given determinantal element is written $\phi_{k_m}(r_n)=\exp(ik_mr_n)$. For a one-dimensional system of N total electrons of L sites, a stationary configuration has wave vectors $k_m=(2m-1-N)\pi/L$ for the F and G fields and $k_m=(2m-1-N/2)\pi/L$ for each determinant in S. Because N is always even, the F and G obey antiperiodic boundary conditions. The field S has periodic (antiperiodic) boundary conditions for an odd (even) number of up or down electrons. Alone, S is the ground state of the noninteracting ($U=0$) limit of the Hubbard model.

We emphasize that single-particle basis functions other than plane waves may be chosen as has been done with the GW.[1,2] In particular, simple mean-field analysis in two dimensions indicates that a commensurate flux phase[12,13] in the F and G fields coupled with a plane-wave S field may stabilize at certain filling fractions.

A second mean-field decoupling of the composite particle Hamiltonian is possible in which we condense the auxiliary Fermi fields into a single Bose field. We make the substitution $b_i^{\dagger}=f_i^{\dagger}g_i^{\dagger}$, and rewrite the Hamiltonian (3) with auxiliary bosons as

$$H_b^{\text{MF}}=-t\sum_{\langle ij\rangle\sigma}(\langle s_{i\sigma}^{\dagger}s_{j\sigma}\rangle\langle b_i^{\dagger}b_j\rangle+\text{H.c.})\,. \tag{6}$$

Our composite operator is now $c_{i\sigma}^{\dagger}=s_{i\sigma}^{\dagger}b_i^{\dagger}$. The $b_i^{\dagger}$ obey Bose commutation relations for operators on different sites, but Fermi relations for same-site operators, thus ensuring the hard-core nature. Again, we require that the composite particles be "tied" to one another, or $s_{i\sigma}^{\dagger}s_{i\sigma}=b_i^{\dagger}b_i$.

Hard-core bosons in a one-dimensional system can be transformed into Fermi operators by the Jordan-Wigner transformation:[14]

$$a_j^{\dagger}=b_j^{\dagger}\exp\left[i\pi\sum_{i<j}b_i^{\dagger}b_i\right]\,, \tag{7}$$

where the $a_j^{\dagger}$ now obey Fermi statistics. So we may write our auxiliary boson wave function as

$$\Psi_b=\Theta(r_j^{\uparrow},r_j^{\downarrow})\;F(r_j^{\uparrow},r_j^{\downarrow})\;S(r_j^{\uparrow},r_j^{\downarrow}) \tag{8}$$

where the new function

$$\Theta(r_i)=\prod_{i<j}\text{sgn}(r_i-r_j) \tag{9}$$

due to the transformation (7) preserves the overall Fermi statistics of the wave function. Note that Θ has antiperiodic boundary conditions for an even total particle number, so the boundary convention used for Ψ_f is applicable here.

Since H_f is effectively a mean-field approximation of H_b, we expect Ψ_b to be superior at approximating the exact behavior. However, in higher-dimensional systems,

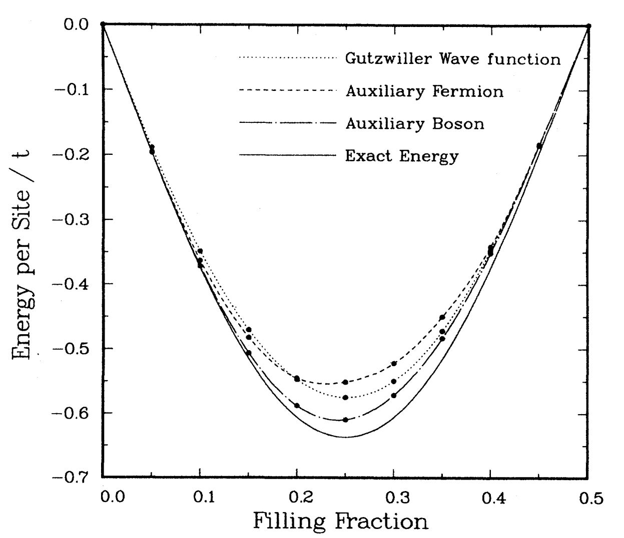

FIG. 1. A comparison of the ground-state energy per site as a function of filling fraction. The auxiliary fermion formulation exceeds the Gutzwiller wave function for low filling fractions up to about 0.2, while the auxiliary boson is the best approximation for all fillings. The system size is 100 sites.

the transformation from hard-core Bose operators into modified Fermi operators is no longer as simple, and it may be easier to deal directly with Ψ_f.

To evaluate the ground-state expectation values of the energy and other observables for our trial wave functions we employ the "inverse update" Monte Carlo sampling method discussed by Ceperley, Chester, and Kalos,[15] and used with great success for the GW.[1,2] We emphasize that except for the necessity of evaluating an extra determinant for the auxiliary fields, our wave functions are just as simple to evaluate in this manner as the usual GW.

The energy of our wave functions as a function of electron filling is shown in Fig. 1. We have plotted for comparison the exact result from the Bethe ansatz and the GW energy. As expected, Ψ_b yields a lower kinetic energy than Ψ_f for all band fillings, and at low density both methods are superior to GW. The physics behind this improvement is clear: Gutzwiller projection introduces a "sharp" correlation hole of one lattice spacing, which raises the kinetic energy. Our composite states produce a much smoother correlation hole with a density-dependent breadth and a long-range oscillatory tail. However, the product nature of our wave functions tends to overcorrelate the electrons, costing energy. This is especially true for Ψ_f, the product of three determinants, and for filling fractions above approximately 0.2, the GW energy is lower than that of Ψ_f. As one approaches the half-filled band, however, it is clear that our procedure is forced to generate an "on-site" projector, identical to Gutzwiller, and we see the methods converge numerically.

We determine the momentum distribution $n(k)$ by transforming the real-space single-particle density matrix in the usual way:

$$n(k) = \langle c_{k\sigma}^{\dagger} c_{k\sigma} \rangle = \frac{1}{L} \sum_{ij} \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle \exp[ik(r_i - r_j)] \quad (10)$$

for a system of L sites. As in the calculation of the energy, we implement the local constraint $s_{i\sigma}^{\dagger} s_{i\sigma} = f_i^{\dagger} f_i = g_i^{\dagger} g_i$ exactly in our calculation of $n(k)$.

The momentum distribution of Ψ_b, Ψ_f, and the GW for the quarter-filled system are shown in Fig. 2. The GW exhibits a discontinuity at k_F and rises for $k > k_F$, with no unusual behavior at $3k_F$. The exact Bethe ansatz solution has a power-law singularity near k_F obeying the relation

$$n(k) = n(k_F) - C|k - k_F|^{\alpha} \operatorname{sgn}(k - k_F) \quad (11)$$

with $\alpha = \frac{1}{8}$.[8-10] Fitting our data to this form, we find $\alpha_b = 0.27 \pm 0.01$ and $\alpha_f = 0.58 \pm 0.02$. Additionally, we see evidence of the singularity at $3k_F$ that exists in the exact solution.

Finally, in Fig. 3 we plot the z component of the spin-correlation functions for the quarter-filled band, defined by

$$S^z(k) = \frac{1}{L} \sum_{ij} \langle S_i^z S_j^z \rangle \exp[ik(r_i - r_j)] \,. \quad (12)$$

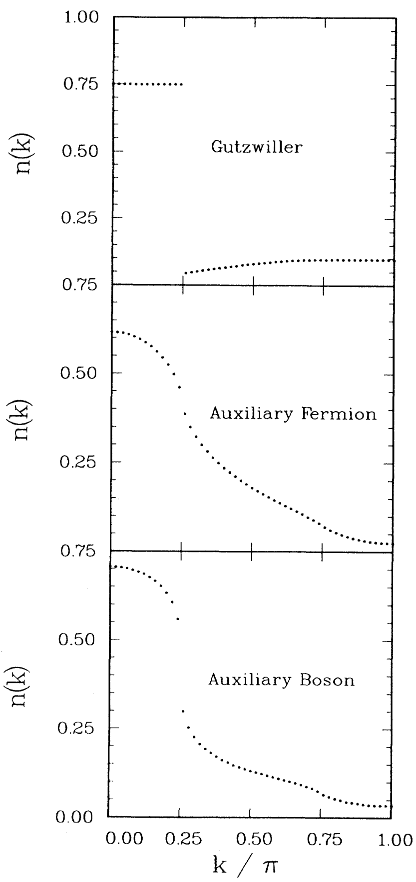

FIG. 2. The momentum distributions $n(k)$ for the quarter-filled band. The Gutzwiller wave function exhibits a discontinuity at $k_F = \pi/4$ and is an increasing function above k_F. Both composite particle formulations exhibit power-law singularities at k_F and weak singularities at $3k_F$. The system size is 100 sites.

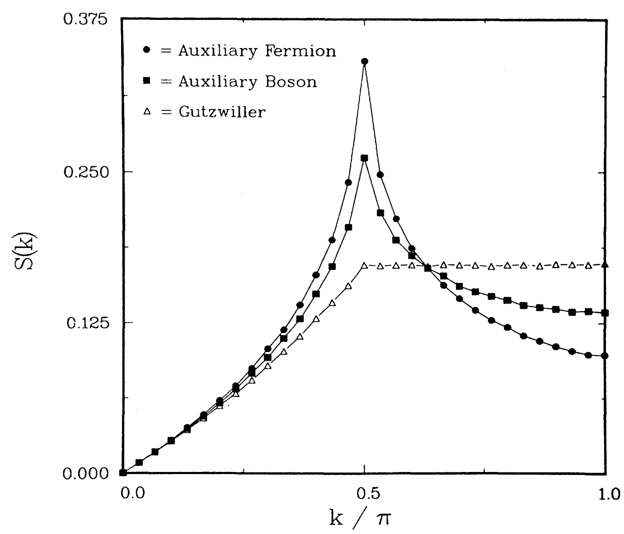

FIG. 3. The spin-correlation functions for the quarter-filled band. The height of the cusp at $2k_F = \pi/2$ differs greatly between the different formulations: The auxiliary boson formulation has the correct height within statistical errors, while the auxiliary fermion overcorrelates and the Gutzwiller wave function undercorrelates. The system size is 60 sites.

The power-law cusp at $2k_F = \pi/2$ is absent in the GW. The height of the cusp predicted by the auxiliary boson formulation of $S^z(2k_F) = 0.262 \pm 0.008$ agrees within errors with the exact results from the Bethe ansatz.[8] The auxiliary fermion formulation tends to overcorrelate the electrons, and it overestimates the height at $2k_F$.

The utility of the procedure is that it can readily be boosted to higher dimensions, and we are currently working in this direction. As mentioned above, mean-field calculations in two dimensions with the auxiliary fermion wave function indicate that a commensurate flux phase can stabilize at certain fillings. Additionally, hard-core bosons in two dimensions exhibit off-diagonal long-range order at zero temperature,[16] so we may be able to generate wave functions with true Fermi surfaces in our auxiliary boson formulation.

In application of the method to the one-dimensional t-J model we have found that simple wave functions of this form to a remarkably complete job of reproducing the ground-state phase diagram in the J/t-n plane.[17,18]

In summary, we have developed a variational wave function for the strongly correlated Hubbard model in arbitrary dimension that is very tractable computationally and superior to the Gutzwiller wave function at estimating the energy and correlation functions in one dimension.

This work was supported by National Science Foundation Grant No. DMR 90-08256.

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