Ground-State Properties of Correlated Fermions: Exact Analytic Results for the Gutzwiller Wave Function

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The properties of the Gutzwiller variational wave function, which is frequently used to study ground-state properties of correlated fermions with a short-range interaction, are investigated by use of a new, analytically tractable approach. As a first application several ground-state quantities are evaluated exactly in dimension $d=1$ for arbitrary band filling and interaction strengths. The results allow for the first approximation-free assessment of the wave function. The method itself is applicable to arbitrary space dimensions.

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Correlated Fermi systems play a particularly important role in physics. However, they are also known to be notoriously difficult to tackle. In condensed-matter physics the theoretical investigations of the unusual properties of "heavy-fermion systems"[1] have further intensified the efforts to understand the effects of strong interactions among fermions. The difficulties involved are well known from the theory of narrow-band metals[2] and liquid ^{3}He.[3,4] They are all examples of systems with a strong, short-range repulsive interaction between the respective spin-$\frac{1}{2}$ fermions. This type of correlation is often approximated by a Hubbard-type, i.e., on-site, interaction[5,6]:

$$H_I = U\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where $n_{i\sigma}=c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator for fermions with spin σ on a lattice at site i. Such a term is therefore part of many model Hamiltonians constructed to describe the correlations between fermions.[1-4,7,8] In the simplest case the interaction part H_I may be supplemented by a kinetic part

$$H_{\rm kin} = \sum_{i,j,\sigma} t_{ij}c_{i\sigma}^\dagger c_{j\sigma} = \sum_{\mathbf{k},\sigma}\epsilon_{\mathbf{k}}n_{\mathbf{k}\sigma}, \tag{2}$$

where $t_{ij}=L^{-1}\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}\exp[i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)]$ is a general hopping matrix element, L is the number of lattice sites, and $n_{\mathbf{k}\sigma}$ is the momentum distribution operator. In the special case of nearest-neighbor hopping, $H=H_{\rm kin}+H_I$ is commonly referred to as the Hubbard model.[5,6] In spite of the exact solution of this model in $d=1$ dimension,[9] properties for $d>1$ are hardly understood. While numerical methods[10] have already yielded important insight, manageable analytic methods would clearly be particularly desirable. To this end variational methods, which generally go beyond perturbation theory, have found widespread application.

In particular, the variational wave function first suggested by Gutzwiller,[5]

$$|\psi_{\rm G}\rangle = \prod_i[1-(1-g)D_i]\,|\psi_0\rangle, \tag{3}$$

has been extensively used to study ground-state properties of Hamiltonians containing the interaction term (1). Here $D_i=n_{i\uparrow}n_{i\downarrow}$, $|\psi_0\rangle$ is the noninteracting, paramagnetic ground state, and the correlation parameter g, $0\le g\le 1$, acts as a variational parameter. The purpose of the correlation factor in $|\psi_{\rm G}\rangle$ is to reduce the weight of spin configurations with doubly occupied sites in $|\psi_0\rangle$, i.e., to suppress local charge (i.e., density) fluctuations. As such it may be expected to be particularly suited for the investigation of higher-dimensionality systems. In spite of the simplicity of Eq. (3), exact analytical evaluations of expectation values valid for arbitrary correlation strength in the thermodynamic limit have not yet been feasible. Nevertheless, investigations of finite systems, i.e., of one-dimensional rings, by Kaplan, Horsch, and Fulde[11] and by Horsch and Kaplan[12] have already provided valuable insight into the properties of the Gutzwiller wave function. Hashimoto[13] used similar findings to obtain approximations for higher-dimensionality systems in the thermodynamic limit. Furthermore, results for the thermodynamic limit have been obtained by perturbational calculations[7,8,13,14] and by employing Gutzwiller-type approximations.[5,15,16] Most recently, Gros, Joynt, and Rice[17] and Yokoyama and Shiba[18] have presented detailed numerical calculations of several quantities in terms of the Gutzwiller wave function.

In this Letter we outline a new approach to the calculation of expectation values of an operator O,

$$\langle O\rangle = \langle\psi_{\rm G}|O|\psi_{\rm G}\rangle/\langle\psi_{\rm G}|\psi_{\rm G}\rangle,$$

which is both simple and analytically tractable. It is valid for arbitrary correlation strengths g, particle densities n, and space dimensions d.

Expanding $|\psi_G\rangle$ in (3) as a sum over lattice sites $\mathbf{f}_i$, the calculation of $\langle H_I\rangle$ is seen to involve the evaluation of expectation values,

$$x_m = \sum_{\mathbf{f}_1,\ldots,\mathbf{f}_m}' \langle D_{\mathbf{f}_1}\cdots D_{\mathbf{f}_m}\rangle_0, \quad m \le L,$$

with $\mathbf{f}_i \ne \mathbf{f}_j$ (prime on sum) in the noninteracting ground state. Wick's theorem transforms $\langle\cdots\rangle_0$ into $\{\cdots\}_0$, the sum over all pairs of "contractions" defined by $\{c^\dagger_{i\sigma}c_{j\sigma}\}_0 \equiv \langle c^\dagger_{i\sigma}c_{j\sigma}\rangle_0$ ($\equiv P_{ij}$ in Refs. 7 and 8) and, in particular, $\{c_{j\sigma}c^\dagger_{i\sigma}\}_0 \equiv -P_{ij}$. Note that in the latter case the usual δ_{ij} term does *not* appear; hence

$$x_m = \sum_{\mathbf{f}_1,\ldots,\mathbf{f}_m}' \{D_{\mathbf{f}_1}\cdots D_{\mathbf{f}_m}\}_0.$$

However, $\{\cdots\}_0=0$ for any $\mathbf{f}_i=\mathbf{f}_j$ since then two rows in the corresponding determinant are equal. One may therefore *extend the summation over all* $\mathbf{f}_i$, i.e.,

$$x_m = \sum_{\mathbf{f}_1,\ldots,\mathbf{f}_m} \{D_{\mathbf{f}_1}\cdots D_{\mathbf{f}_m}\}_0.$$

The x_m can be represented diagrammatically with lines corresponding to $P_{\mathbf{f}_i,\mathbf{f}_j}$. Since disconnected diagrams cancel the norm $\langle\psi_G|\psi_G\rangle$, one is left with

$$x_m^c = \sum_{\mathbf{f}_1,\ldots,\mathbf{f}_m} \{D_{\mathbf{f}_1}\cdots D_{\mathbf{f}_m}\}_0^c,$$

the connected diagrams contributing to x_m. In the case of $\langle H_I\rangle$ we have

$$\langle H_I\rangle = ULg^2\sum_{m=1}^{\infty}(g^2-1)^{m-1}c_m, \tag{4}$$

with $c_m = x_m^c/L(m-1)!$. The expression for $\langle H_I\rangle$ is different from that of Gutzwiller[5,16] since it only involves connected diagrams. In particular it differs from the one obtained by previous investigations[7,8,14] based on the "linked cluster method,"[19] where the correlation factor in (3) is written as $e^{-\eta D}$, with $\eta=\ln(1/g)$ and $D=\sum_i D_i$. In the latter approach weak correlations ($g \lesssim 1$) are treated by use of η, rather than $1-g^2$, as an expansion parameter. In this case the different c_m are mixed, which makes a general evaluation of $\langle H_I\rangle$ untractable. In $d=1$ it is easy to show that $c_m \propto n^{m+1}$, where $n=N/L\le 1$ is the density of particles and $n_\uparrow=n_\downarrow=n/2$. With use of the n dependence of $\langle H_I\rangle$, particle-hole symmetry, and the continuity of the first derivative with respect to n at $n=1$, the prefactor can be calculated. One obtains the general expression[20]

$$c_m = \tfrac{1}{2}(-1)^{m+1}n^{m+1}/(m+1). \tag{5}$$

In the thermodynamic limit ($L\to\infty$) the expectation value of H_I is then found as

$$\langle H_I\rangle = L\frac{Un^2}{2}\left[\frac{g}{1-G^2}\right]^2\left[\ln\frac{1}{G^2}+G^2-1\right], \tag{6}$$

where $G^2=1-n+ng^2$. Hence for a half-filled band ($n=1$) the correlation term is found to be *nonanalytic* in g. In particular, for strong correlations ($g\to 0$) $\langle H_I\rangle = LUg^2\ln(1/g)$. The logarithmic correction to the g^2 dependence is unexpected. It is also difficult to observe in a numerical analysis where $\langle H_I\rangle$ appears quadratic in g.[18] The density of doubly occupied sites is given by $d=\langle H_I\rangle/UL$. For $1\le n\le 2$, $d(n)=d(2-n)+n-1$ by particle-hole symmetry.

To obtain the expectation value of the kinetic energy one has to calculate the one-particle density matrix $G_{i,j,\sigma}=\langle c^\dagger_{i\sigma}c_{j\sigma}\rangle$, whose Fourier transform is the momentum distribution

$$\langle n_{\mathbf{k}\sigma}\rangle = [1-(1-g)^2 n_{-\sigma}]n^0_{\mathbf{k}\sigma} + \frac{1}{(1+g)^2}[1-(1-g^2)n^0_{\mathbf{k}\sigma}]\sum_{m=2}^{L}(g^2-1)^m f^{(m)}_{\mathbf{k}\sigma}, \tag{7}$$

where $n^0_{\mathbf{k}\sigma}$ is the momentum distribution of the noninteracting system and $f^{(m)}_{\mathbf{k}\sigma}=h^{(m)}_{\mathbf{k}\sigma}+c_{m-1}$, with

$$h^{(m)}_{\mathbf{k}\sigma} = -\frac{1}{L}\frac{1}{(m-2)!}\sum_{\mathbf{f}_1,\ldots,\mathbf{f}_m} e^{-2\pi i\mathbf{k}\cdot(\mathbf{f}_2-\mathbf{f}_1)}\{c_{\mathbf{f}_1\sigma}n_{\mathbf{f}_1,-\sigma}D_{\mathbf{f}_3}\cdots D_{\mathbf{f}m}n_{\mathbf{f}_2-\sigma}c^\dagger_{\mathbf{f}_2\sigma}\}_0^c. \tag{8}$$

The functions $f^{(m)}_{\mathbf{k}\sigma}$ may be represented by connected graphs carrying an external momentum $\mathbf{k}$, with lines corresponding to factors $n^0_{\mathbf{k}\sigma}$ and $n^0_{\mathbf{k}-\sigma}$ and with point vertices. Their structure is identical to the usual mth order, connected Green's function for point interactions.[21] These diagrams are expressible in terms of irreducible graphs $f^{(m)}_{\mathbf{k}\sigma,\mathrm{irr}}$. The $f^{(m)}_{\mathbf{k}\sigma}$ have a discontinuity at $|\mathbf{k}|=k_\mathrm{F}$ because they include reducible graphs, i.e., carry single, reducible lines, and therefore vanish for $|\mathbf{k}|>k_\mathrm{F}$. By contrast, the $f^{(m)}_{\mathbf{k}\sigma,\mathrm{irr}}$ are continuous functions of the momentum across k_F with $f^{(m)}_{\mathbf{k}\sigma}=f^{(m)}_{\mathbf{k}\sigma,\mathrm{irr}}$ for $|\mathbf{k}|>k_\mathrm{F}$. In $d=1$ dimension, this property, together with particle-hole symmetry for $n=1$, yields a recursion relation between the two functions. For $n_\uparrow=n_\downarrow=n/2$, one finds ($n\le 1$)

$$f^{(m)}_{k_{\mathrm{F}-}} = (-1)^m[(2m-1)!!/(2m)!!]n^m, \tag{9}$$

and $f^{(m)}_{k_{\mathrm{F}-},\mathrm{irr}}=f^{(m)}_{k_{\mathrm{F}-}}/(2m-1)$, where $k_{\mathrm{F}-}=k_\mathrm{F}-0$. In this way $\langle n_{\mathbf{k}\sigma}\rangle$ may be calculated at $k=k_\mathrm{F}\pm 0$. One finds that $\langle n_{k_{\mathrm{F}+}}\rangle=\frac{1}{2}[(1-G)/(1+g)]^2$ and $\langle n_{k_{\mathrm{F}-}}\rangle = q + \langle n_{k_{\mathrm{F}+}}\rangle$, where q is the discontinuity of $\langle n_k\rangle$ at the Fer-

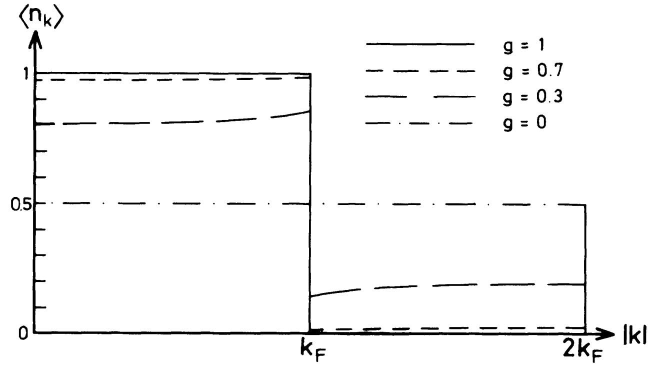

FIG. 1. The momentum distribution $\langle n_{\mathbf{k}}\rangle$ for several values of the correlation parameter g in the case of a half-filled band ($n_\uparrow = n_\downarrow = \frac{1}{2}$).

mi surface,

$$q = G^{-1}[(G+g)/(1+g)]^2. \tag{10}$$

The numerical results of Ref. 18 are found to be in excellent agreement with this approximation-free evaluation. For $n=1$ one has $q = 4g/(1+g)^2$, the result of the Gutzwiller *approximation.*[16] Equation (10) implies the existence of a Fermi surface for correlation parameters $0 < g \leq 1$ in the case of a half-filled band. [We have obtained a similar result in $d=2$ dimension and expect it to be true for arbitrary dimensions since our derivation of (7) is quite general.]

Equation (7) may be used to calculate $\langle n_{k\sigma}\rangle$ in a power series in terms of $1-g^2$. To this end the quantities $f_{\mathbf{k}\sigma}^{(m)}$ have to be calculated. In $d=1$ dimension they are polynomials in k and n. The use of particle-hole symmetry and the continuity of the first two derivatives of $f_{\mathbf{k}\sigma}^{(m)}$ with respect to n at $n=1$ yields enough equations to generate the $f_{\mathbf{k}\sigma}^{(m)}$ recursively.

For correlations $0 < g < 1$, $\langle n_{\mathbf{k}\sigma}\rangle$ is seen to increase slightly both for $|\mathbf{k}| < k_F$ and $|\mathbf{k}| > k_F$ (see Fig. 1) in contrast to what one should expect. This feature agrees with the numerical results for small[13] and large[17,18] finite systems. At $k_F \pm 0$, $\langle n_{\mathbf{k}\sigma}\rangle$ is found to be nonanalytic in the limits $n \to 1$, $g \to 0$. The kinetic energy $E_{\text{kin}}(g) = L^{-1}\langle H_{\text{kin}}\rangle$ may now be calculated for given ϵ_k. For strong correlations ($g \to 0$), one finds that

$$E_{\text{kin}}(g) = E_{\text{kin}}(0) + 2g[\bar{\epsilon}_0 - E_{\text{kin}}(0)],$$

where $\bar{\epsilon}_0 = L^{-1}\sum_\sigma \sum_{|\mathbf{k}| < k_F} \epsilon_k$ is the average kinetic energy in the noninteracting system. In particular, for $n_\uparrow = n_\downarrow = \frac{1}{2}$, this yields $E_{\text{kin}}(g) = 2g\bar{\epsilon}_0$. For nearest-neighbor hopping (Hubbard model) $\epsilon_k = -2t\cos(2\pi k)$ and $\bar{\epsilon}_0 = -4t/\pi$. After minimization with respect to g, the ground-state energy E of the Hubbard model is obtained. For $n=1$ and $U \to \infty$ one finds

$$E = -(4/\pi)^2(t^2/U)(\ln\bar{U})^{-1}, \tag{11}$$

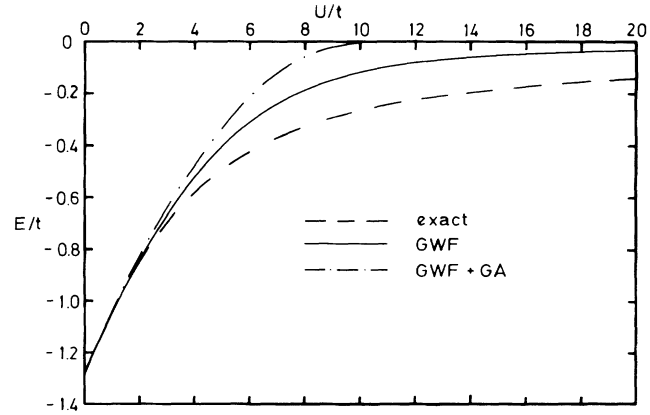

FIG. 2. The ground-state energy E for the one-dimensional Hubbard model with $n_\uparrow = n_\downarrow = \frac{1}{2}$ as a function of U. The results for E, as calculated with the Gutzwiller wave function (GWF), are compared with the result of the Gutzwiller approximation (GWF+GA) (Ref. 23) and the exact result (Ref. 9).

where $\bar{U} = U/|\bar{\epsilon}_0|$, i.e., E is *nonanalytic* in $t/U \to 0$. Hence in the thermodynamic limit the wave function $|\psi_G\rangle$ does not lead to a $(-t^2/U)$ dependence known from the exact result.[9,22] This is in contrast to earlier conclusions based on the extrapolation of the results for finite systems, where the logarithmic correction in Eq. (11) cannot be identified and hence is interpreted as a (small) prefactor to a $(-t^2/U)$ dependence.[11] Kaplan, Horsch, and Fulde[11] therefore discussed an improvement of (3) which yielded a much better numerical agreement with the ground-state energy of the exact result.[9] With use of Eq. (7) and the results for $f_{\mathbf{k}\sigma}^{(m)}$, one may calculate the ground-state energy E in $d=1$ dimension. For $n=1$, the result is shown in Fig. 2, in comparison with the exact result[9] and the Gutzwiller approximation.[16]

The above results for the discontinuity q imply the existence of a Fermi surface for the interacting fermions of the Hubbard model in $d=1$ dimension at any finite U and for $n \leq 1$. (Hence a Mott transition does not take place at any finite U.) While the exact $\langle n_{\mathbf{k}}\rangle$ for $n=1$ is not expected to show a discontinuity for $U > 0$,[24] a Fermi surface may well exist for $n < 1$, and the results for $\langle n_{\mathbf{k}}\rangle$ obtained with the Gutzwiller wave function indeed show such a feature. In higher dimensions and for lattices without perfect nesting, even the exact solution for $n=1$ is expected to exhibit a Fermi surface at small U, in which case a Brinkman-Rice–type transition,[23] where the discontinuity q vanishes at a finite U, has to occur.

In view of the above results obtained with $|\psi_G\rangle$ for the Hubbard model, one might conclude that, at least in $d=1$ dimension, the Gutzwiller wave function was not a good variational *Ansatz,* particularly for $U \to \infty$. However, this conclusion is unwarranted. In fact, our approach also yields analytic results for the correlation functions,[25] e.g., the spin- and density-correlation function, for arbitrary g and n. For infinitely strong interaction and $n=1$ the former exhibits antiferromagnetic correlations in excellent agreement with exact results. This was already observed in numerical studies.[11,12,17,18]

In conclusion, we have presented an analytical approach to the calculation of ground-state properties of correlated fermions with the Gutzwiller wave function. It allows one to perform the exact evaluation of several expectation values in $d=1$ dimension. As such, it allows for the first unambiguous assessment of the Gutzwiller wave function. The method may also be applied to higher space dimensions. In particular, we have found strong indications that the Gutzwiller approximation[16] becomes exact in the limit $d \rightarrow \infty$.

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