

Analytic Calculation of Momentum Distributions and Ground State Energies of Correlated Fermions with the Gutzwiller Wave Function

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A new analytic approach is discussed which allows for an exact evaluation of ground state properties of correlated fermions in terms of the Gutzwiller variational wave function in $d = 1$. The results are applied to the Hubbard model. The approach may also be used to investigate higher dimensional systems.

The problems involved in the investigation of Fermi systems with a strong, short-range repulsive interaction is complex enough to defy analytic solutions in all but very special cases. In the absence of simple, reliable perturbative approaches, variational methods prove to be very helpful. In order to study the so-called Hubbard-model [1,2], a lattice model for itinerant fermions with an on-site interaction $H_I = U \sum_i D_i$ (here $D_i = n_{i\uparrow} n_{i\downarrow}$ is the number operator for double occupancy of a lattice site), Gutzwiller introduced a simple variational wave function [1]

$$|\psi_G\rangle = \prod_i [1 - (1-g)D_i] |\psi_0\rangle \quad (1)$$

Based on the non-interacting system with wave function $|\psi_0\rangle$, the prefactor in (1) is supposed to reduce the amplitude of spin configurations in $|\psi_0\rangle$ with too many sites on which the interaction takes place. Here $0 \leq g \leq 1$ is a variational parameter. Although $|\psi_G\rangle$ is extremely simple, exact evaluations of expectation values $\langle X \rangle = \langle \psi_G | X | \psi_G \rangle / \langle \psi_G | \psi_G \rangle$ could not be performed until recently - not even in the case of H_I , to which $|\psi_G\rangle$ is custom-tailored, or in $d = 1$ dimension. Expansions [3], Gutzwiller-type approximations [4] and numerical techniques [5-9] had to be used instead, which altogether elucidated several of the properties of $|\psi_G\rangle$. Most recently Metzner and Vollhardt [10] presented a new analytic approach to calculate expectation values with $|\psi_G\rangle$. It applies to arbitrary dimensions d and is particularly simple in $d = 1$, where the shape of the Fermi "surface" is independent of the band filling $n = N/L \leq 1$ ($L =$ number of lattice sites). This fact allows for exact, analytic evaluations in $d = 1$, e.g. of ground state properties [10] and correlation functions [11] for Hubbard-type models. We illustrate the method in the case of $\langle H_I \rangle$. Expanding (1) one may construct expectation values

$$x_m = \sum_{\vec{f}_1 \dots \vec{f}_m} \langle D_{f_1} \dots D_{f_m} \rangle_0 \quad (2)$$

in the non-interacting ground state, where all site indices \vec{f}_i are different. As usual

Wick's theorem transforms $\langle \dots \rangle_0$ into $\{ \dots \}_0$, the sum over all pairs of contractions, where the usual term $\delta_{\vec{f}_i, \vec{f}_j}$ never occurs because $\vec{f}_i \neq \vec{f}_j$ by construction. On the other hand, $\{ \dots \}_0 = 0$ for any $\vec{f}_i = \vec{f}_j$. Hence, on summing over the \vec{f}_i the restriction $\vec{f}_i \neq \vec{f}_j$ may be dropped which yields

$$x_m = \sum_{\vec{f}_1 \dots \vec{f}_m} \{ D_{f_1} \dots D_{f_m} \}_0 \quad (3)$$

The x_m may be presented diagrammatically, where lines correspond to factors $\langle n_{k\sigma} \rangle_0$ and where the disconnected diagrams cancel the norm $\langle \psi_G | \psi_G \rangle$. This leaves us with x_m^c , the connected diagrams of (3). In the case of $\langle H_I \rangle$ for $d = 1$ we have

$$\langle H_I \rangle = U L g^2 \sum_{m=1}^L (g^2 - 1)^{m-1} c_m$$

where $c_m = [L(m-1)!]^{-1} x_m^c \propto n^{m+1}$; here we assumed $n_\uparrow = n_\downarrow = n/2$. Using particle-hole (ph) symmetry at $n = 1$ the precise form of c_m is calculated as [10]

$$c_m = \frac{(-n)^{m+1}}{2(m+1)} \quad (4)$$

such that ($L \rightarrow \infty$)

$$\langle H_I \rangle = \frac{LU}{2} \left(\frac{g^2}{1-g^2} \right) \left[\ln \frac{1}{G^2} + G^2 - 1 \right] \quad (5)$$

where $G^2 = 1 - (1-g^2)n$. Eq. (5) is non-analytic in the limit $g = 0, n = 1$.

The momentum distribution $\langle n_{k\sigma} \rangle$ is more difficult to calculate owing to the external parameter k . It is obtained as [10]

$$\langle n_{k\sigma} \rangle = [1 - (1-g)^2 n_{-\sigma}] \langle n_{k\sigma} \rangle_0 + \frac{1}{(1+g)^2} [1 - (1-g^2) \langle n_{k\sigma} \rangle_0] \sum_{m=2}^{\infty} (g^2 - 1)^m f_{k\sigma}^{(m)}, \quad (6)$$

where the $f_k^{(m)}$ correspond to connected graphs with m vertices (as in the case of the c_m), which now carry an external momentum k . Their topological structure is identical to that of the usual m^{th} -order connected Green functions. In $d = 1$ their actual values are given by polynomials in $|k|$ and n which are different for $k \lesssim k_F$. Differentiability with respect to n and ph-symmetry at $n = 1$ allows one to calculate

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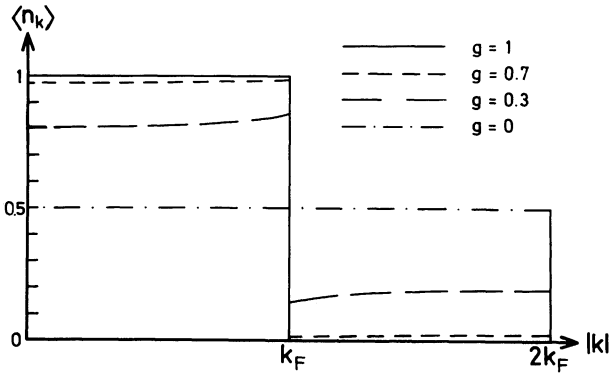


Fig. 1. The momentum distribution $\langle n_k \rangle$ for different correlation parameters g at $n = 1$.

the $f_{k\sigma}^{(m)}$ recursively. In this way $\langle n_{k\sigma} \rangle$ is obtained as shown in Fig. 1. For $g > 0$ there is a discontinuity at k_F (sharp Fermi surface) which only vanishes at $g = 0$. Above and below k_F , $\langle n_k \rangle$ has a slight upward cusp, i.e. the k -dependence is opposite to what one should expect. The size $q = \langle n_{k_F-0} \rangle - \langle n_{k_F+0} \rangle$ of the discontinuity may be calculated from (6). To this end the functions $f_{k_F \pm 0}^{(m)}$ have to be determined at $k = k_F \pm 0$, where $k_F = \pi n/2$. In this special case $f_{k_F \pm 0}^{(m)} \propto n^m$ with different coefficients for $k_F \pm 0$. Differentiability with respect to n and ph -symmetry for $n = 1$ yields

$$f_{k_F-0}^{(m)} = (-n)^m \frac{(2m-1)!!}{(2m)!!} \quad (7)$$

$$f_{k_F+0}^{(m)} = f_{k_F-0}^{(m)} / (2m-1).$$

Hence $\langle n_{k_F+0} \rangle = \frac{1}{2} [(1-g)/(1+g)]^2$ and

$$q = \frac{1}{g} \left[\frac{g+g}{1+g} \right]^2 \quad (8)$$

For $n = 1$ we find $g = 4g/(1+g)^2$, which holds in arbitrary dimensions d . We note that this approximation-free result is identical to that of the Gutzwiller-approximation [1,4] which we find to be correct in $d = \infty$. Hence $|\psi_G\rangle$ always leads to a Fermi surface except for $g = 0$.

The above results may be directly applied to diagonalize the Hubbard-model in terms of $|\psi_G\rangle$ with an arbitrary kinetic energy ϵ_k . For strong correlations and $n = 1$.

$$E_{kin} = \frac{2}{L} \sum_k \epsilon_k \langle n_k \rangle = 2g \bar{\epsilon}_0,$$

where $\bar{\epsilon}_0$ is the average kinetic energy for $g = 1$. For next-neighbor hopping and after minimization with respect to g the ground

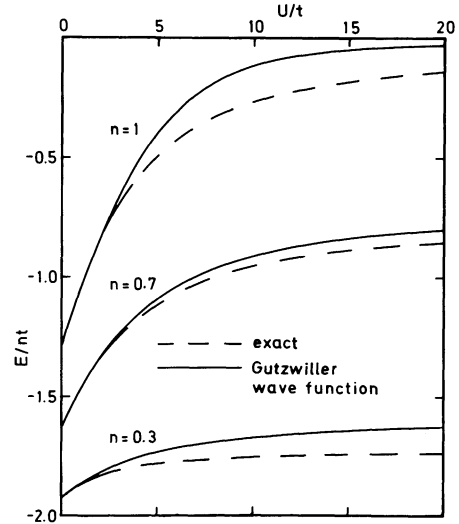


Fig. 2. The ground state energy per particle of the $d = 1$ Hubbard-model for different densities, as compared with the exact results [12].

state energy of the Hubbard-model is found. For large U

$$E = -\left(\frac{4}{\pi}\right)^2 \frac{t^2}{U} \frac{1}{\ln \bar{U}}, \quad (9)$$

where $\bar{U} = U/|\bar{\epsilon}_0|$. The logarithmic term in (9) makes E quite a bit higher than the exact result [12], which has a $(-t^2/U)$ -dependence for large U . Its origin seems to lie in the missing correlation between doubly occupied and empty sites in $|\psi_G\rangle$ [11] - a fact, which was already realized earlier [5] on the basis of numerical calculations. In Fig. 2 we show the ground state energy per particle of the Hubbard model for different densities as obtained with $|\psi_G\rangle$ in comparison with the exact results [12].

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