Interacting Fermions: Correlation Functions Obtained with the Gutzwiller Wave Function

Florian GEBHARD*
Physik Department, T 30, Technische Universität München, D-8046 Garching, F.R. Germany
Dieter VOLLHARDT*
Max-Planck-Institut für Physik und Astrophysik, D-8000 München 40, F.R. Germany

A recently developed analytic approach is used to calculate correlation functions for interacting spin-1/2 fermions on a lattice in terms of the Gutzwiller wave function. In one dimension the evaluations are performed analytically and without any approximation. Whenever possible comparison with exact results (Hubbard-model, spinless fermions) is made.

The well-known difficulties involved in the theoretical treatment of interacting Fermi systems, especially those with a strong, short-range repulsive interaction, have made variational methods particularly attractive [1]. In order to study a lattice model of itinerant electrons with an on-site interaction [2,3,4] ("Hubbard-model") Gutzwiller [2] introduced a variational wave function |ψG⟩, which controls local (on-site) density fluctuations in the ground state wave function of the non-interacting fermi gas, |ψ0⟩,

\[ |ψ_G⟩ = \prod_i (1-(1-μ)D_i)|ψ_0⟩ \]  

where \( D_i = n_i^+ n_i^- \) is the number operator for double-occupation of a lattice site ("D-site") and \( 0 \leq g \leq 1 \) is a variational parameter. The projection operator in (1) merely reduces the number of D-sites (where the interactions occur) of the spin contributions contributing to |ψ0⟩. It is simple in structure, exact evaluations of expectation values \( \langle X \rangle \sim \langle X |ψ_G⟩/\langle ψ_G|ψ_G⟩ \) of an operator \( X \) have not been possible for a long time. Therefore expansion techniques [4], mean field-type approximations [5] and numerical methods were employed [6-9]. Most recently, however, a new, analytically tractable approach to the problem was developed by Metzner and Vollhardt [10], which is based on a somewhat unconventional combination of Wick's theorem and well-known diagrammatic techniques. Expectation values are expressed as a series in powers of \( 1-g^2 \), whose coefficients can be calculated to any order - at least in one dimension. In higher dimensions numerical methods have to be used. In this way the ground state energy of the d=1 Hubbard-model in terms of |ψG⟩ has been obtained without approximation [10].

We now go on to calculate correlation functions (CFs) [11]. In lattice models with itinerant up/down spins a site may be occupied by single spins, D-sites and empty sites ("holes"). Introducing number operators at site \( i \) for the spin \( S_i^+ = n_i^+ - n_i^- \), density \( N_i = n_i^+ + n_i^- \), D-sites \( D_i = n_i^+ n_i^- \) and holes \( H_i = (1-n_i^+)(1-n_i^-) \) we want to calculate the CFs

\[ C_{j}^{XY} = \frac{1}{L} \sum_{l=1}^{L} (\langle \psi | X_{l}^† Y_{l} | \psi \rangle - \langle \psi | \psi \rangle \langle \psi | X | \psi \rangle - \langle \psi | Y | \psi \rangle) \]  

where \( j \) is the number of lattice sites, \( X = L^{-1} \sum \chi_i \) etc. and \( \chi_i = \sigma_i^1 \chi_i, \sigma_i^0 \), \( \chi_i \). This defines 10 CFs. For \( n_1 = n_2 = n/2 \), with \( n = N/L \leq 1 \) as the particle density, there remain only seven, four of which are independent. We choose \( C_{SS}^S, C_{NN}, C_{HH} \) and \( C_{DB} \) since they have a direct physical significance. We note that for \( x = y \) the \( \bar{q} = 0 \) limit of the Fourier transform of (2), \( C_{XX}(\bar{q}=0) = \langle X^† X \rangle - \langle X \rangle^2 \), is a measure for the fluctuations in the number \( \langle X \rangle \) around its average. In the present case, where a fixed number of particles \( \langle N \rangle = n \) and a total spin \( \langle S^z \rangle = 0 \) is considered, \( C_{SS}(\bar{q}=0) = C_{NN}(\bar{q}=0) = 0 \), while \( C_{DD}(\bar{q}=0) = 0 \) because there is no conservation law for D-sites or holes. -

In the following we limit our discussion to \( d = 1 \) dimension and \( n = 1 \) unless stated otherwise.

1) The spin-CF \( C_{SS}^S \) is of particular interest, because the results obtained with (1) may be compared with the exact results for \( j = 1,2 \) in the d = 1 Hubbard-model in the atomic limit [12]. One obtains \( C_{SS}^S(q) = (1-g^2)^2 kF(q) \) where \( F(x) = 1-(1-g^2)x \) and \( q = |q|/r \). In the atomic model \( q = 0 \), \( C_{SS}^S(q=2k_F) \) is seen to diverge logarithmically, implying an anti-ferromagnetic transition. In real space

\[ C_{S}^{j} = \frac{1}{f(y)} \frac{1}{y} \int_{0}^{1} dy \sin(\pi j y) \frac{2}{f(y)} \frac{\sin(\pi j y)}{\pi j} \]  

so that for \( g = 0 \) one finds

\[ C_{S}^{j} |_{g=0} = (-1)^j \frac{\sin(\pi j)}{\pi j} \]  

In Fig. 1 \( C_{S}^{j} \) is plotted for different values of the correlation parameter \( g \). The \((-1)^j/j\) dependence has already been suggested earlier [7]. The numerical calculations for \( j = 1 \) [6-8] and \( j = 2 \) [7] are seen to be very accurate. The results obtained from (4) are also in very good agreement with exact [12] and numerical [13] results for the antiferromagnetic Heisenberg chain. Hence we see that for \( n = 1 \) the Gutzwiller wave function describes spin correlations in the interacting system very well.

*Address as of Oct. 1, 1987: Institut für Theoretische Physik C, Technische Hochschule Aachen, 5100 Aachen, FRG.
2) The density-CF is found as $\rho_{NN}(q) = \frac{g^2}{(1-g^2)} | \rho_{NN}(Q)/g^2 |$. The additional $g$-factor, as compared to $\rho_{SS}$, reflects the suppression of density fluctuations for $g \to 0$.

3) For $g = 0$ and $n < 1$ holes act as spinless fermions whose number is conserved [8]. In this limit the hole-CF $\rho_{HH}$ is given by $\rho_{HH} = \rho_{NN}^g = \rho_{NN}^g$, while its exact value is given by $\rho_{HH}^n$ with $n \rho_n$ replaced by the hole concentration $n_H = 1 - n$ and $k_F^B = n_H$, respectively. It turns out [11] that $\rho_{HH}$ obtained with $|\psi_G\rangle$ describes the overall features of the exact result (correlation hole of width $1/n_H$, oscillations etc.) very well as was already concluded from Monte-Carlo calculations [8].

4) For $n = 1$ the CF between D-sites and holes is given by $\rho_{DH} = \rho_{HH} - \frac{1}{2} \rho_{NN}$, such that for $g = 0$ $\rho_{DH}(q) = -\frac{1}{2} \rho_{NN}(q)$. Since correlations in (1) merely tend to smooth out the distribution of particles on the lattice, the latter result implies that there is only an average correlation between D-sites and holes, resembling the non-interacting case. In Fig. 2 we show $\rho_{DH} = \rho_{DH}(q) + q^2)/d$, the probability for finding a hole at distance $j$ from a D-site, normalised to the non-interacting case, which clearly shows this feature. On the other hand, for strong interactions this probability should be higher than in the uncorrelated case, because this would make a decay of a high-energy D-site easier. As discussed earlier [6] the lack in spatial correlation appears to be the main origin for the rather high ground state energy of the $d = 1$ Hubbard-model obtained with $|\psi_G\rangle$ at strong interactions $U$, which is caused by logarithmic corrections to the usual $-t^3/U$-dependence [10].

The above results may be directly used to diagonalize Hubbard-type models with more complicated than on-site interactions. -

We thank W. Metzner for useful discussions.

REFERENCES

10) W. Metzner and D. Vollhardt, MPI-preprint PFA/Ph 14/87.
11) F. Gebhard and D. Vollhardt, MPI-preprint PFA/Ph 29/87.