Interacting Fermions: Correlation Functions Obtained with the Gutzwiller Wave Function

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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] ("Hubbard-model") Gutzwiller [2] introduced a variational wave function $|\psi_G\rangle$, which controls local (on-site) density fluctuations in the ground state wave function of the non-interacting Fermi gas, $|\psi_o\rangle$,

$$|\psi_G\rangle = \prod_i [1-(1-g)D_i]|\psi_o\rangle \qquad (1)$$

Here $D_i = n_{i\uparrow}n_{i\downarrow}$ is the number operator for double occupancy of a lattice site ("D-site") and $0 \le g \le 1$ is a variational parameter. The projection operator in (1) merely reduces the number of D-sites (where the interactions occur) of the spin configurations contributing to $|\psi_o\rangle$.- Athough $|\psi_G\rangle$ is simple in structure, exact evaluations of expectation values $\langle X\rangle = \langle\psi_G|X|\psi_G\rangle/\langle\psi_G|\psi_G\rangle$ 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 $|\psi_G\rangle$ 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 ($S_i^z = n_{i\uparrow} - n_{i\downarrow}$), density ($N_i = n_{i\uparrow} + n_{i\downarrow}$), D-sites ($D_i = n_{i\uparrow}n_{i\downarrow}$) and holes ($H_i = (1-n_{i\uparrow})(1-n_{i\downarrow})$) we want to calculate the CFs

$$C_j^{XY} = \frac{1}{L}\sum_i \langle X_i Y_{i+j}\rangle - \langle X\rangle\langle Y\rangle \qquad (2)$$

where L is the number of lattice sites, $X = L^{-1}\sum_i X_i$ etc. and $X_i, Y_i = S_i^z, N_i, D_i, H_i$. This defines 10 CFs. For $n_\uparrow = n_\downarrow = n/2$, with $n = N/L \le 1$ as the particle density, there remain only seven, four of which are independent. We choose C^{SS}, C^{NN}, C^{HH} and C^{DH} since they have a direct physical significance. We note that for X = Y the $\vec{q} = 0$ limit of the Fourier transform of (2), $C^{XX}(q=0) = \langle X^2\rangle - \langle X\rangle^2$, 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, $C^{SS}(\vec{q}=0) = C^{NN}(\vec{q}=0) = 0$, while $C^{DD}(\vec{q}=0) \neq 0$ 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_j^{SS} 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 $C^{SS}(q) = -(1-g^2)^{-1}\ln F(Q)$ where $F(x) = 1-(1-g^2)x$ and $Q = |q|/\pi$. In the atomic (g = 0), $C^{SS}(q=2k_F)$ is seen to diverge logarithmically, implying an anti-ferromagnetic transition. In real space

$$C_j^{SS} = -\frac{1}{\pi j}\int_0^1 dy\, \frac{\sin(\pi j y)}{F(y)}\,, \; j > 0 \qquad (3)$$

so that for g = 0 one finds

$$C_j^{SS}\Big|_{g=0} = (-1)^j \frac{Si(\pi j)}{\pi j} \qquad (4)$$

In Fig. 1 C_j^{SS} 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.

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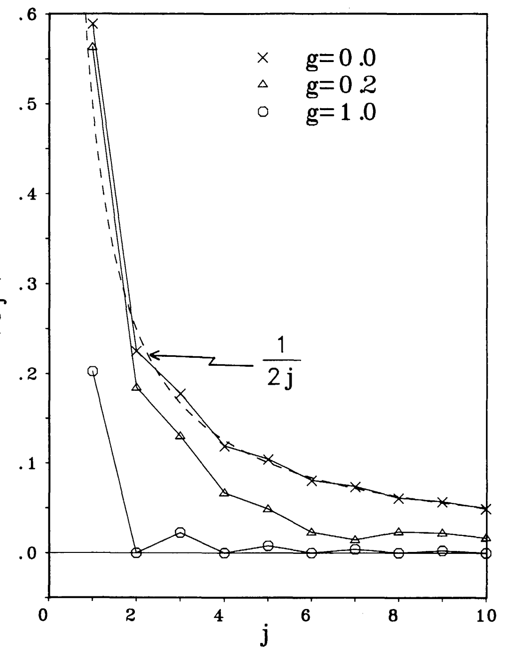

Fig 1. The magnitude of the spin-correlation function C_j^{SS} vs. separation j for different correlation parameters g.

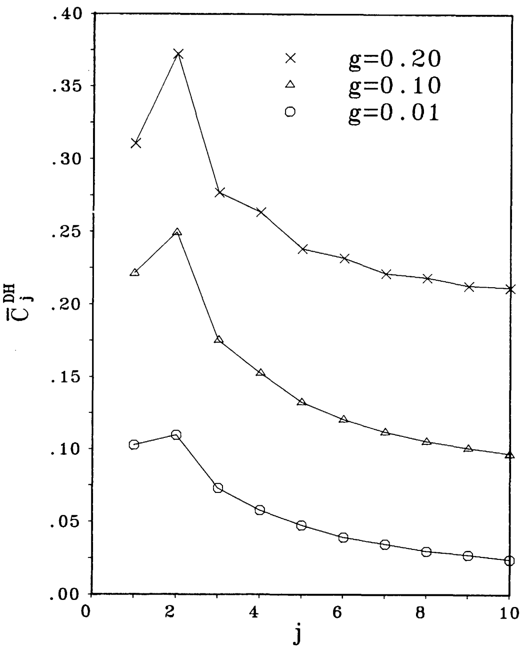

Fig. 2. The probability for finding an empty site at separation j from a doubly occupied site, normalized to the non-interacting case, for different correlation parameters g.

2) The density-CF is found as $C^{NN}(q) = [g^2/(1-g^2)]\ell nF(-Q/g^2)$. The additional g^2-factor, as compared to C^{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 C^{HH} is given by $C^{HH}_{g=0} = C^{NN}_{g=0}$, while its exact value is given by $C^{HH}_{g=1}$ with n, k_F replaced by the hole concentration $n_h = 1-n$ and $k_F^h = \pi n_h$, respectively. It turns out [11] that $C^{HH}_{g=0}$ obtained with $|\psi_G\rangle$ describes the overall features of the exact result (correlation hole of width $1/2n_h$, 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 $C^{DH} = C^{HH} - \frac{1}{2} C^{NN}$, such that for $g \to 0$ $C^{DH}(q) \simeq -\frac{1}{2} C^{NN}(q)$. Since correlations in (1) merely tend to smoothen 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 $\tilde{C}_j^{DH} = (C_j^{DH} + d^2)/d$, 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 $-t^2/U$-dependence [10].

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

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