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VARIATIONAL WAVE FUNCTIONS FOR CORRELATED LATTICE FERMIONS

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INTRODUCTION

Variational wave functions (VWFs) are among the very few theoretical tools that allow for straightforward, conceptually simple investigations of interacting many-body systems. They are used to describe correlations among quantum mechanical objects in an approximate, but explicit and physically intuitive,manner. They are particularly valuable in situations where standard perturbation theory fails or is not tractable. The problems in which VWFs have been employed include such diverse examples as rotons in superfluid ^{4}He [1], the plasma state of electrons in metals [2], the quantum liquids ^{3}He and ^{4}He [3-5], nuclear physics [6], superconductivity [7] and the fractional Quantum-Hall-Effect [8]. Of these the BCS-wave function is certainly the most famous. VWFs have also been used to study the possibilities for magnetic order of lattice electrons, i.e. ferromagnetism [9] and antiferromagnetism. [10-11]

At present VWFs receive a renewed interest due to the investigations of heavy fermion systems [12] and high-T_c superconductivity [13], which involve strongly correlated lattice electrons. In the absence of exact solutions of the models used for their description, e.g. the periodic Anderson model, the Hubbard model and its extentions and the Heisenberg model, VWFs provide a valuable and tractable method to study the limit of strong interactions, which is so difficult to investigate otherwise. This is clearly also reflected in the large number of groups around the world (most notably in Danmark, France, Hungary, Italy, Japan, Switzerland, USA and West-Germany) involved in such studies. In the following I will discuss the structure of variational wave functions and their applications to strongly correlated Fermi systems. Special attention is given to recent developments in the variational investigation of the Hubbard model and the antiferromagnetic Heisenberg model in reduced dimensions. Finally, a summary of the exact analytic results available today in d=1 and/or d=∞ for the simplest of these variational wave functions - the Gutzwiller wave function - and generalizations thereof will be presented.

APPLICATION TO QUANTUM LIQUIDS (^{3}He, ^{4}He)

The quantum liquids ^{3}He and ^{4}He are of particular interest in many-body physics since they represent the prototypes of Fermi (^{3}He)- and Bose (^{4}He)-liquids. In contrast to electronic systems they are neutral and extremely pure liquids, which are composed of only a single species. Microscopically ^{3}He is much more complicated than ^{4}He due to the antisymmetry of the wave function, as required by the Pauli-principle. On the other hand, Fermi statistics allows at the same time for the formulation of a very powerful phenomenological theory of Fermi liquids, namely Landau's Fermi liquid theory[14], which is not available in a Bose system. It is the existence of a Fermi surface (if it exists), which allows for well-defined elementary excitations, i.e. quasi particles, and which thereby renders possible a complete description of the low-temperature properties of a Fermi liquid (for details see ref. 15).

Microscopic investigations aiming at an understanding of the quasiparticle interaction use a combination of many-body perturbation theory, variational methods and Monte-Carlo calculations (see Krotscheck, ref. 5). These approaches have the advantage of working with systems in the thermodynamic limit and hence are independent of the size of the system. Over the last 30 years they seem to have developed into a science all by itself. The idea behind the variational method is based on the Jastrow-Feenberg approach[3-6] of constructing a VWF $|\psi>$ by applying a correlation operator $\hat{C}$ on a suitably chosen one-particle starting wave function $|\phi_0>$

$$|\psi> = \hat{C}|\phi_0> \tag{1}$$

The operator $\hat{C}$ contains the interaction between the particles in parametrized form, i.e. describes it by variational parameters. It may be expressed as

$$\hat{C} = \exp\left\{ \sum_{i<j} u_2(r_{ij}) + \sum_{i<j<k} u_3(r_{ij}, r_{ik}) + \ldots \right\} \tag{2}$$

where $r_{ij}=r_i-r_j$, and the first term in the exponential corresponds to two-body terms, the second to three-body terms etc. These describe the purely geometrical correlations of the short-ranged hard core interaction. In addition, state dependent (e.g. spin-)interactions have to be included. Alternatively, one can write

$$\hat{C} = \left[\prod_{ij} f_2(r_{ij}) \right] \left[\prod_{ijk} f_3(r_{ij}, r_{ik}) \right] \left[S \prod_{ij} (1 + \lambda_{ij}\, \sigma_i \sigma_j) \right] \ldots \tag{3}$$

where now such a state dependent interaction has been explicitly included, with S as a symmetry operator. The wave function $|\psi>$ for the interacting system is then constructed by suitably enhancing those configurations in $|\phi>$ which are most important, i.e. which contain the favorable correlations. In this way the wave function may be adjusted. An important task is then to calculate the expectations values of on operator $\hat{O}$

$$<\hat{O}> = \frac{<\psi|\hat{O}|\psi>}{<\psi|\psi>} \tag{4}$$

Most important is $\hat{O} = \hat{H}$, with $\hat{H}$ as the Hamiltonian, such that the ground state energy can be evaluated. To this end cluster expansions and self-consistent summation techniques are employed ("Hypernetted Chain Theories").[3 - 6] Clearly, the VWF $|\psi\rangle$ should contain sufficient local correlations but must still be tractable.

Among the techniques employing a combination of variational methods and many-body perturbation theory the "Correlated Basis Function" (CBF)-Theory is most successful.[3 - 6] It is designed to improve the ground state wave function and describe the excited states at the same time, using a non-orthogonal basis $\{|\psi_m\rangle\}$, where

$$|\psi_m\rangle = \hat{C}|\phi_m\rangle \tag{5}$$

is constructed by letting $\hat{C}$ act on an independent particle basis $\{|\phi_m\rangle\}$. The ground state energy

$$E\{\lambda_i\} \equiv \langle \hat{H} \rangle \tag{6}$$

will depend on explicit variational parameters λ_i, with respect to which E has to be minimized

$$\frac{\delta E}{\delta \lambda_i}\Big|_{\bar{\lambda}_i} = 0 \tag{7}$$

This leads to an upper bound for the exact ground state energy E_0

$$E_0 \leqslant E\{\bar{\lambda}_i\} \tag{8}$$

A serious problem is that usually the energy alone is not a sensitive indicator for the quality of the VWF. The advantage of using a VWF is, however, that it is very physical and that it allows for direct improvements guided by physical requirements. In the case of liquid ^{3}He - being an enormously difficult system - one may say that although detailed quantitative agreement with experiment is still lacking, the overall progress has been remarkable and great amount of underlying physics has been understood .[5]

CORRELATED ELECTRONS

In contrast to Helium-atoms electrons are pointlike particles. It is therefore very important to distinguish between models in which electrons are confined to a lattice ("lattice models") and those in which they can move continuously in space ("continuum models"). In the latter case electrons may move in such a way as to avoid each other, which makes the bare interaction effectively much softer. Furthermore, a point-interaction (δ-function potential) has no effect at all in dimensions $d > 2$,[16] i.e. the particles simply do not see each other. Therefore in $d = 3$ a point-like δ-function potential is unphysical. In lattice models this is different. The lattice sites provide definite points where the interaction takes place. Therefore on a lattice even point-like particles have a finite probability for interaction, independent of the dimension of the lattice. In this way strong on-site interactions are possible.

As discussed in the introduction, VWFs designed to describe electronic systems are wellknown from standard mean field theories (e.g. Hartree-Fock) for weakly interacting (quasi-) particles. The most famous is the BCS-wave function,[7] which in its most general form (including anisotropic pairing) is given by [17]

$$|\psi_{BCS}> = \prod_{k} \prod_{\sigma} [u_{k,\sigma\sigma} + \sum_{\sigma'} v_{k,\sigma\sigma'} \hat{a}^{\dagger}_{k\sigma} \hat{a}^{\dagger}_{-k\sigma'}] \quad (9)$$

Here $\hat{a}^{\dagger}_{k\sigma}$ creates a particle with momentum $\mathbf{k}$ and spin σ and the 2 x 2 spin matrices $\underline{u}_k$, $\underline{v}_k$ are to be determined variationally. On the other hand, the developments in the theory of heavy fermions and high-T_C superconductivity have clearly indicated the need for an explicit inclusion of (i) the lattice, and, (ii) strong, short-range repulsive interactions. In this respect elementary mean field theories and VWFs are clearly insufficient. The generic model which takes such features explicitly into account by concentrating on the bare essentials, is the Hubbard model[18-20]

$$\hat{H}_{Hub} = \hat{H}_{kin} + \hat{H}_{int} \quad (10)$$

with

$$\hat{H}_{kin} = \sum_{ij} \sum_{\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \quad (11a)$$

$$= \sum_{k} \sum_{\sigma} \varepsilon_k \hat{n}_{k\sigma} \quad (11b)$$

$$\hat{H}_{int} = U \sum_{i} \hat{n}_{i\downarrow} \hat{n}_{i\uparrow} \quad (12a)$$

$$= U \hat{D} \quad (12b)$$

where $c^{\dagger}_{i\sigma}(c_{i\sigma})$ creates (destroys) a fermion at site i with spin σ and $\hat{n}_{i\sigma}=\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$ is the number operator. The first term, $\hat{H}_{kin}$, is the kinetic energy which describes the hopping of spins from site j to site i; it is thus of purely quantum mechanical origin. Using the momentum representation, this term may equally be expressed as shown in (11b), where ε_k is the energy dispersion and $\hat{n}^{\dagger}_{k\sigma} = \hat{a}^{\dagger}_{k\sigma}\hat{a}_{k\sigma}$ is the momentum distribution operator with $\hat{a}^{\dagger}_{k\sigma}(\hat{a}_{k\sigma})$ as creation (annihilation) operators for particles with momentum $\mathbf{k}$ and spin σ. The Hubbard interaction $\hat{H}_{int}$, (12), is purely on-site and is essentially classical: it only contributes if two particles with opposite spin occupy the same lattice site. As written in (12b) this term therefore gives the total number of doubly occupied sites, $\hat{D}$, of the system, with $\hat{D} = \Sigma_i \hat{D}_i$ and $\hat{D}_i = \hat{n}_{i\downarrow}\hat{n}_{i\uparrow}$. Clearly, due to the presence of $\hat{H}_{kin}$ the ground state wave function is not an eigenfunction of $\hat{D}$. In the special case of nearest neighbor hopping we can choose $t \equiv 1$, such that

$$\hat{H}_{Hub} = \sum_{<ij>} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U\hat{D} \quad (13)$$

Hence, at T = 0 the Hubbard model depends on one parameter U; for U = 0 it describes free lattice fermions and for U = ∞ localized spins.

There is another model of considerable interest - interesting in its own right - namely the Heisenberg model, describing localized Heisenberg spins S_i with a nearest neighbor coupling

$$\hat{H}_{Heis} = J \sum_{<ij>} S_i \cdot S_j \tag{14}$$

Clearly, this overall coupling constant J is arbitrary and may just as well be fixed, e.g. $J \equiv 1$. Therefore this model and its wave function depend on no parameter at all.- For half filling ($n_\uparrow = n_\downarrow = n/2$, $n = 1$) and $U \to \infty$ the Hubbard model and the Heisenberg model are related. This may be shown by second order perturbation theory[21] or, equivalently, by applying a unitary transformation to the Hubbard Hamiltonian (13) and demanding the absence of doubly occupied sites.[22] This leads to

$$\hat{H}_{eff} = -t \sum_{<ij>} \sum_{\sigma} (1 - \hat{n}_{i,-\sigma}) \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} (1 - \hat{n}_{j,-\sigma}) + \frac{4t^2}{U} \sum_{<ij>} (\hat{S}_i \cdot \hat{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j) + \hat{H}_3 \tag{15}$$

Here the first term describes the hopping of holes, i.e. of empty sites, and $\hat{H}_3$ contains processes involving three particles. In the second part one has

$$S_i = \hat{c}_i^{+} \sigma \hat{c}_i \tag{16}$$

where

$$\hat{c}_i^{+} = \begin{pmatrix} \hat{c}_{i\uparrow}^{+} \\ \hat{c}_{i\downarrow}^{+} \end{pmatrix}, \quad \hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \tag{17}$$

and $\sigma = \tau/2$ with τ as the Pauli matrices. For half-filling the first and third term vanish and, apart from a constant ($\hat{n}_i \hat{n}_j \to 1/4$), $\hat{H}_{eff}$ reduces to (14), where now the constant J is uniquely determined by the parameters of the Hubbard model as

$$J = \frac{4t^2}{U} \tag{18}$$

It may seem puzzling at first that at large, but still finite U, the Hubbard model, which always contains hopping of particles and thereby a finite number of doubly occupied sites, is related to the Heisenberg model, describing strictly localized spins. The reason is that for $U \to \infty$ doubly occupied sites in the Hubbard model become <u>virtual</u>, their density decreasing as $d \propto (t/U)^2$, such that their contribution to the ground state energy is of order t^2/U. This process is contained in J. For smaller U the two models are sufficiently different; therefore they require very different kinds of VWFs for their description.

In spite of many decades of work on these models the number of exact results for the thermodynamic limit is exceedingly small- even for ground state properties. Only in d=1 dimension is the ground state energy[23] and the spin correlation function[24] of the Heisenberg model known (and thereby that of the half-filled Hubbard-model for large U and nearest [23] and next-nearest[25] neigbors). Everything else (i.e. the explicit wave functions, other correlation functions, the momentum distribution in the case of the Hubbard model etc.)

is unknown even in d = 1 and the situation is, of course, even much worse in higher dimensions.

In this situation VWFs are one of the very few tools at hand that allow for theoretical investigations of strongly correlated many-body fermion systems. Since the Hubbard model is the generic model describing strong on-site correlations, the question is how to incorporate their effects in VWFs for this model. An important approach, which is widely used at present, goes back to Gutzwiller[9,18], who constructed a VWF (the "Gutzwiller wave function" $\hat{=}$ GWF) $|\psi_G\rangle$

$$|\psi_G\rangle = g^{\hat{D}}|FS\rangle \tag{19a}$$

$$= \prod_i [1-(1-g)\hat{D}_i]\,|FS\rangle \tag{19b}$$

where

$$|FS\rangle = \prod_{|k|<k_F} \hat{a}^\dagger_{k\uparrow}\hat{a}^\dagger_{k\downarrow}\,|0\rangle \tag{19c}$$

is the Fermi sea with $|0\rangle$ as the vacuum, and the operator $g^{\hat{D}}$, with $0 \leqslant g \leqslant 1$ as a variational parameter, reduces the amplitude of those spin configurations in $|\phi_0\rangle$ which at a given interaction U contain too many doubly occupied sites. This may also be interpreted in a different way: by noting the projection property $\hat{n}^2_{i\sigma} = \hat{n}_{i\sigma}$, the density fluctuation operator $\hat{N}^2$ is written as

$$\frac{1}{2}\hat{N}^2 = \frac{1}{2}\sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})^2 = \frac{1}{2}\hat{N} + \hat{D} \tag{20}$$

Thus, for fixed particle number

$$g^{\hat{D}} \sim g^{\frac{1}{2}\hat{N}^2} \tag{21}$$

stating that $g^{\hat{D}}$ suppresses density fluctuations in a <u>global</u> sense.

The GWF (19) has precisely the Jastrow-Feenberg form discussed above, with $g^{\hat{D}}$ being the correlation operator which controls the main effect of the strong correlations, i.e. the suppression of double occupancies. This wave function may in principle be refined and adapted to specific physical situations by either generalizing the correlation operator itself, or - as will be discussed below - by putting the details into the starting wave function $|\phi_0\rangle$ such that

$$|\psi\rangle = g^{\hat{D}}|\phi_0\rangle \tag{22}$$

i.e. generalizing (19) to a more detailed form. Examples for VWFs containing $g^{\hat{D}}$ on top of a refined starting wave function $|\phi_0\rangle$ are

$$|\psi_{G,\,PAM}\rangle = g^{\hat{D}} \prod_{k,\sigma} [1 + a(k,\sigma)\,\hat{f}^\dagger_{k\sigma}\hat{c}_{k\sigma}]\,|FS\rangle \tag{23}$$

as is used for the periodic Anderson model.[26-30] Here $|\phi_0\rangle$ introduces a hybridization between the f-electrons and the conduction electrons, while $g^{\hat{D}}$ controls the number of sites doubly occupied by f-electrons. Another example is

$$|\psi_{G,\,AFHF}> = g^{\hat{D}} \prod_{k,\sigma} [u_{k\sigma}\, \hat{c}^{\dagger}_{k\sigma} + \sigma v_{k,\,\sigma}\, \hat{c}^{\dagger}_{k-Q,\,\sigma}]|0> \qquad (24)$$

where $|0>$ is the vacuum. This VWF has been investigated in detail by Yokoyama and Shiba[31,32]. Here $|\phi_0>$ is the usual wave function used to obtain the anti-ferromagnetic Hartree-Fock (AFHF) approximation for the Hubbard model[10,11], $u_{k\sigma}, v_{k\sigma}$ are variational functions and $Q = (\pi, \ldots \pi)$ is half the reciprocal lattice vector for the square lattice. The factor $g^{\hat{D}}$ improves the energy for small U which otherwise is non-analytic.

Probably the most wellknown of such VWFs is the "resonating valence bond" (RVB) state suggested by Anderson[33,34] in 1973 as a possible ground state of the antiferromagnetic spin-½ Heisenberg model for a two-dimensional, triangular lattice. It is made up of singlets on sites i and j

$$\hat{b}^{\dagger}_{ij} = \frac{1}{\sqrt{2}} (\hat{c}^{+}_{i\uparrow}\, \hat{c}^{+}_{j\downarrow} - \hat{c}^{+}_{i\downarrow}\, \hat{c}^{+}_{j\uparrow}) \qquad (25)$$

which are then superimposed. For a distribution of bond lengths a linear combination has the form

$$\hat{b}^{+} = \sum_{k} a(k)\, \hat{c}^{\dagger}_{k\uparrow}\, \hat{c}^{\dagger}_{k\downarrow} \qquad (26)$$

where $\Sigma_k\, a(k) = 0$ to avoid double occupancy. The RVB-state then has the form

$$|\psi_{RVB}> = \lim_{g\to 0}\; g^{\hat{D}}\, (\hat{b}^{+})^{N/2}|0> \qquad (27a)$$

which may equivalently be written as

$$|\psi_{RVB}> = \lim_{g\to 0}\; g^{\hat{D}}\, \hat{P}_{N/2}\, [u_k + v_k \hat{c}^{\dagger}_{k\uparrow}\, \hat{c}^{+}_{-k\downarrow}]\,|0> \qquad (27b)$$

Clearly, $|\psi_{RVB}>$, (27), is a special form of the BCS-wave function (9), namely with exactly N/2 spin-singlet Cooper pairs. Note that the GWF, (19), is <u>also</u> a special case of $|\psi_{RVB}>$, (27a), namely that with $a(k) = 1$ for $k < k_F$, $a(k) = 0$ for $k > k_F$. In particular, following the proposal by Anderson[35], the RVB-wave function is used as a starting point for investigations of high-T_c superconductivity[13] in the two-dimensional Hubbard-model (plus its various extentions), when holes have been introduced to allow for hopping of the "preexisting" Cooper-pairs. So $|\psi_{RVB}>$ generalizes the BCS-wave function to a lattice model where double occupancy has to be eliminated in view of the strong on-site interactions. It is interesting to note that the need for a somewhat similar generalization of $|\psi_{BCS}>$ has been felt in the case of superfluid ^{3}He,[17] where Cooper pairs are made up of ^{3}He-atoms which strongly interact via a hard core interaction. As discussed by Leggett[36] a more realistic Cooper pair wave function than the model form used within BCS-theory should be employed, with the central part being effectively cut out. - The (resonating) valence bond approach is also wellknown in chemical physics where it is used for the representation of molecular structure.[37]

We see that, in principle, one may introduce more and more refinements into the GWF by custom tayloring it to the specific situation involved. However, this also creates problems: the evaluations of expectation values is becoming more and more difficult. Analytic calculations of the strongly correlated regime, if possible at all, only seem to be tractable in d = 1 anyhow (and in d = ∞, see below). On the other hand, numerical techniques - in particular variational Monte Carlo methods - are always limited to finite systems and are only able to determine a finite number of variational parameters. They cannot, in general, determine entire functions which usually appear in VWFs.

RECENT DEVELOPMENTS

In the last few years - and particularly most recently in the wake of high-T_c activities - substantial progress has been made in the refinement of VWFs described above. Here the great advantage of VWFs becomes evident, namely their explicit nature, which allows for direct improvements guided by physical insight. In most cases the evaluation of expectation values in terms of a given VWF has to be done numerically.

Important improvements of the GWF were first discussed by Stollhoff and Fulde[38] in their calculations of correlation energies of moleculs. They used a wave function containing density-density type, i.e. local, correlations between neighboring sites

$$|\psi\rangle = \prod_i \left[\prod_j (1 - \eta_i \sum_{\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j+i,\sigma'}) \right] |FS\rangle \qquad (28)$$

where the variational parameters η_i are explicitly site dependent - a generalization suitable for finite systems. Thereby excellent correlation energies can be obtained, making this ansatz a very good approach for molecules etc. - Applying a similar idea to a VWF for the Hubbard model in d=1 Kaplan, Horsch and Fulde[39] generalized the GWF by introducing an additional variational parameter h which controls the number $\langle\hat{Q}\rangle$ of holes and doubly occupied sites sitting on neighboring sites

$$|\psi\rangle = g^{\hat{D}} h^{\hat{Q}} |FS\rangle \qquad (29)$$

They had found that in the GWF, in particular for strong correlations, such pairs where not kept close enough together, thereby making it hard for a doubly occupied site to dissociate again. - In the group of Rice at the ETH-Zürich detailed numerical investigations of the effective Hamiltonian (15) have been performed. Gros, Joynt and Rice[22] obtained accurate numerical evaluations of the spin-spin and hole-hole correlation functions in d = 1 in terms of the GWF. These results yielded important insight into the appropriateness of the GWF. Furthermore, Gros[40] and Zhang, Gros, Rice and Shiba[41] tested the RVB-wave function (25) against the antiferromagnetic state $|\psi_{G,AFHF}\rangle$, (24), in d = 2, finding that in the half-filled case both states are very close in energy, lying about 5% above the estimated ground state. This is astonishing in view of the different

long-range behavior of these two states. This group also investigated the pairing instabilities of generalized GWFs for less than half-filling, finding that a d-wave RVB state is lowest in energy.[40,43] - Parallel to that, but independently, Yokoyama and Shiba[43] obtained similar, very accurate investigations of the Hubbard model, i.e. of the ground state energy, correlation functions, the momentum distribution etc., in terms of the GWF (partly even in d=2,3). They also investigated[31, 32] $|\psi_{G\,,AFHF}>$, (24), for the two-dimensional strongly interacting Hubbard model and compared it with $|\psi_{RVB}>$. The conclusions are similar to those described above obtained by Rice's group (for a comprehensive discussion see ref. 45).- As explained earlier, the RVB-state introduced by Anderson[33,35] is a superposition of singlet-pairs without double occupancy of sites. The general properties of this highly interesting VWF have been discussed in detail by Anderson and co-workers[46-49] in the context of high-T_C superconductivity; within a short time an enormous literature has accummulated (see also ref. 13).

Concerning the ground state of the spin-½ two-dimensional antiferromagnetic Heisenberg model one of the most pertinent questions is whether it possesses long range order or not. This problem has been investigated in detail in terms of VWFs. Horsch and van der Linden[50] constructed a VWF which is a generalization of a state previously considered by Hulthen[23], Kasteleijn[51] and Marshall[52], i.e.

$$|\psi_{HKM}> = \sum_{\text{config.}}' \exp\left[-\eta \sum_{<ij>} (S_i^z S_j^z + \frac{1}{4})\right] \exp(-\eta_c N_c)\,(-1)^{N_A^+} |s_1, \ldots s_N> \tag{30}$$

where the sum includes all configurations with $s_i = \pm ½$ and a total spin $S^z_{tot}=0$. The first exponential suppresses unfavorable spin pairs, the second exponential represents an additional suppression of clusters with equal spin. Both correlation terms act on a starting wave function whose phase is determined by N_A^+, the number of up-spins on the A-sublattice. When writing the ground state wave function in such a way as a superposition of spin-bases, Marshall[52] had proved that the expansion parameters are indeed positive definite - a fact explicitly exploited in (30). The authors found that very good ground state energies could thereby be obtained and that, in particular, this wave function implies long-range order at T = 0, in contrast to the GWF in d = 2.[50] Excited state were also considered. - A similar generalization of the Kasteleijn-Marshall wave function was introduced by Huse and Elser [53]. Their VWF has the form

$$|\psi> = \sum_n e^{\tilde{H}/2} |\psi_n> \tag{31}$$

where $\tilde{H}$ (which contains the variational parameters and which is related to the Hamiltonian under investigation) is an operator diagonal in the complete orthonormal set $\{|\psi_n>\}: \tilde{H}|\psi_n> = \lambda_n|\psi_n>$. Expectation values of an operator $\hat{O}$ may then easily be evaluated by Monte-Carlo. Applying this method, which allows one to include long-range correlations and non-A-B lattices, to the Heisenberg model in d = 2, these authors also find very good ground state energies and, in particular, long range order both for the square and the triangular lattice.[53] - Most recently Tavan[54] presented a

valence bond approach to the Heisenberg-model by representing the lattice in terms of triplet quasiparticles. This leads to a rather simple description of the spin liquid state and its excitations and to a hierarchy of VWFs with very good energies for the ground state in d = 1.

Purely analytic treatments of VWFs for systems in the thermodynamic limit are clearly much more difficult to perform, if possible at all. In particular, the demands on the degree of refinement of the VWF must be much more modest. On the other hand, analytic results are always fixed landmarks which allow for valuable assessments of approximate results. Of all non-mean-field type VWFs for correlated Fermi systems the Gutzwiller wave function (GWF) is the one investigated in greatest detail. Its properties are now very well understood. In spite of its simplicity an exact evaluation of expectation values in terms of the GWF was not possible until recently. Instead, the results of an approximate calculation of the ground state energy, also due to Gutzwiller[9] , were used. In this approximation spatial correlations are neglected. It has been shown to be equivalent to an evaluation of matrix elements by determining the classical statistical weights of different spin configurations in the non-interacting wave function.[55] The Gutzwiller approximation yields very simple results in a number of physical situations (the metal-insulator transition,[56,57] normal liquid ^{3}He[55,58] and heavy fermions[26-30]). It allows to make contact with well established theories like Fermi liquid theory and is therefore generally acknowledged as very "physical", i.e. reasonable. However, to establish the reasonableness of the GWF itself one has to calculate expectation values without making further approximations. Numerical evaluations, first obtained in refs. 22,39,43, have been discussed above. As to analytic approaches Hashimoto[59] used a combination of analytic and numerical methods to obtain improved approximations for one- and higher-dimensional systems in the thermodynamic limit. - Writing the GWF, (19a), as

$$|\psi_G\rangle = e^{-\eta \hat{D}} |FS\rangle \tag{32}$$

where $\eta = \ln(1/g)$, perturbational approaches for $g < 1$ were used by Horsch[60], Baeriswyl and Maki[61] and Baeriswyl, Carmelo and Maki[62] to calculate the ground state energy of the Hubbard model in d = 1 for small interaction strengths U. The momentum distribution n_k was thereby obtained to second order in U.[62] - In the opposite limit, i.e. $U \to \infty$, and for n=1 Baeriswyl[63] suggested the VWF

$$|\psi\rangle = e^{-\lambda \hat{H}_{kin}/t} |\phi_{D=0}\rangle \tag{33}$$

where $|\phi_{D=0}\rangle$ is the wave function containing only those substates of the Fermi sea with no doubly occupied sites and $\hat{H}_{kin}$ is given by (11a) in d = 1. To second order in λ the expectation value of H yields[63]

$$E \simeq (2\lambda t + \lambda^2 U) \frac{\langle\psi|(\hat{H}_{kin}/t)^2|\psi\rangle}{\langle\psi|\psi\rangle} \tag{34}$$

with an optimal value $\lambda = -t/U$. From second-order degenerate perturbation theory we know that the expectation value in (34) is precisely equivalent to that of the spin-½

antiferromagnetic Heisenberg-model. Hence one recovers (14) with $J=4t^2/U$, the exact result in this order. Unfortunately higher orders are very hard to calculate explicitly from (33).-

It would clearly be desirable to be able to perform exact analytic evaluations in terms of such VWFs for <u>arbitrary</u> interaction strengths and particles densities. As shown recently by Metzner and Vollhardt[64] this is indeed possible in the case of the GWF - at least in d = 1 and d = ∞ dimensions. The evaluation is made tractable by (i) a suitable choice of an expansion parameter and (ii) the introduction of special ("δ-less")contractions, which only involve anticommuting numbers. It is essential to note that $\hat{D}_i$ is a purely on-site operator, where all sites i are different. Expressing the expectation value $\langle\hat{O}\rangle$, (4), of an operator $\hat{O}$ in terms of $|\psi_G\rangle$, leads to sums over lattice sites which may be written as sums over <u>different</u> lattice sites only. Thus $\langle\hat{O}\rangle$ takes the form

$$\langle \hat{O} \rangle = \sum_{m=0}^{\infty} 0_m \, (g^2-1)^m \tag{35}$$

where we see that (g^2-1) is the small parameter for expansions around g=1, <u>not</u> $\eta=\ln(1/g)$ as in (32). The coefficients 0_m, which depend explicitly on the density n, may be obtained by standard field theoretic methods where the ensueing contractions only involve anti-commuting numbers as in a Grassmann algebra (a consequence of the lattice sites all being different).[64] In this way it is generally possible to calculate all orders of 0_m in d = 1. Concerning the ground state energy E of the Hubbard model this method allowes one to obtain the expectation values of the momentum distribution $\langle\hat{n}_k\rangle$ and of the Hubbard interaction $\langle\hat{D}\rangle$ without approximation, leading to a E(n,U) for general n and U after minimization w.r.t. to the variational parameter g.[64] - Evaluating the ground state energy of the Hubbard model in d=1 within the hypernetted chain version of the CBF method discussed above (with $\hat{C}$ in (1) corresponding to $g^{\hat{D}}$) Fantoni, Wang, Tosatti and Yu[65] found good agreement with the exact, analytic result.[64]

The above analytic approach has been used by Gebhard and Vollhardt[66] to calculate correlation functions

$$C_j^{XY} = L^{-1} \sum_i \langle\hat{X}_i\hat{Y}_{i+j}\rangle - \langle\hat{X}\rangle \langle\hat{Y}\rangle \tag{36}$$

in terms of $|\psi_G\rangle$ for arbitrary n and U in d=1, where $\hat{X}_i,\hat{Y}_i$ are any one of the four local operators describing the spin $(\hat{S}_i)$, density $(\hat{N}_i)$, empty site $(\hat{H}_i)$ or doubly occupied site $(\hat{D}_i)$ at site i and $\hat{X}=L^{-1}\Sigma_i\hat{X}_i$ etc. Again exact analytic evaluations are possible. In particular, the spin-spin correlation function for n = 1 and U = ∞ is found as

$$C_{j>0}^{ss} = (-1)^j \, \frac{Si(\pi j)}{\pi j} \tag{37a}$$

$$= (-1)^j/2j, \; j\to\infty \tag{37b}$$

The asymptotic behavior implies a logarithmic divergence of the Fourier transform $C^{ss}(q)$ at $q = 2k_F$, i.e. at half a reciprocal lattice vector Q. This antiferromagnetic divergence of $C^{ss}(q=Q)$ is obtained with the GWF in <u>all</u> dimensions d.[66] Comparison with numerical results for C_j^{ss} and the corresponding ground state energy shows that, at least in d=1 and for $U \to \infty$, the GWF is an excellent variational wave function. This conclusion is confirmed by the hole-hole correlations obtained by $|\psi_G\rangle$ for $n < 1$ and $U = \infty$. Recently Haldane[67] and Shastry[68] recognized that the result (38a) is, in fact, the exact result for the continuum Bose gas in d=1, as obtained earlier by Sutherland.[69] Thereby they were able to prove that $|\psi_G\rangle$ is the <u>exact</u> ground state of an $S = \frac{1}{2}$ antiferromagnetic Heisenberg model with $1/r^2$ exchange.

Most recently Metzner and the author[70] showed that exact, analytic evaluations of Hubbard-type models within the GWF are not only possible in d = 1 but also in $d = \infty$. In fact, in this limit VWFs of increasing refinement are found to be analytically tractable without becoming trivial. Diagrammatic evaluations of expectation values in terms of VWFs of the type shown in (22) are greatly simplified in $d = \infty$, since diagrams are made of lines, which correspond to the one-particle density matrix for the non-interacting system $P^0_{ij,\sigma} = \langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle_0$, which obeys

$$P^0_{ij,\sigma} < O\left(\frac{1}{\sqrt{d}}\right) , \quad i \neq j \tag{38}$$

This implies a collapse of those diagrams in which two vertices i and j are connected by three more separate paths, as is the case for the proper self-energy. Exact evaluations of expectation values in $d = \infty$ have sofar been possible for various starting wave functions $|\phi_0\rangle$. In particular, these results show that certain wellknown approximations used previously are exact for specific VWFs in $d = \infty$. Examples are
(i) $|\psi_G\rangle$, eq. (19): In $d = \infty$ the results of the Gutzwiller approximation for the ground state energy are obtained exactly from $|\psi_G\rangle$.[70] Furthermore, correlation functions may be evaluated without approximation.[71] The results have a RPA-type form with a renormalized coupling and show that classical counting arguments for the calculation of <u>next</u> neighbor correlations in terms of $|\psi_G\rangle$ are correct in $d = \infty$.
(ii) $|\psi_{G,AHF}\rangle$, eq. (24): In $d = \infty$ the results of the slave-boson saddle-point approximation applied by Kotliar and Ruckenstein[72] to a functional integral representation of the Hubbard model are recovered.[70] Here we have constructed the explicit <u>wave function</u>, for which this result is exact in $d=\infty$.
(iii) $|\psi_{G,PAM}\rangle$, eq. (23): In $d = \infty$ the results obtained earlier within a Gutzwiller-type approximation,[26-30] based on classical counting arguments, are recovered.[71]

From here one may go on to even more refined VWFs, which still allow for an analytic treatment. Furthermore, 1/d correction can be incorporated to open the way to finite dimensions $1<d<\infty$. Of course, the $d = \infty$ limit is not restricted to the use of VWFs.[70] The method can also be applied to the general many-body Green's function method. The first results obtained for the Hubbard model [73] and the periodic Anderson model[74] are indeed very encouraging.

CONCLUSION

Variational wave functions (VWFs) are one of the most useful and versatile tools for the investigation of strongly correlated Fermi systems. Recently, and within a very short period of time, they have been able to lead to substantial new insight into the properties of low-dimensional lattice systems, such as the Hubbard-, Heisenberg,- and periodic Anderson model. This clearly indicates that there is still a great future potential in this method. New types of VWFs are being investigated and new techniques for their evaluation are devised. To a large extend this is due to the direct, physical nature of VWFs which readily allow for refinements. In this respect it would, for example, be interesting to apply CBF-methods to the investigation of lattice systems to overcome the limitations imposed by working with small, finite systems. Analytic approaches are no longer limited to $d = 1$ dimensions but are now also tractable in $d = \infty$, which opens a new route to the investigation of finite-dimensional systems via $1/d$ expansions. Altogether it is clear that variational wave functions will continue to be an extremely helpful theoretical tool with excellent propects.

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