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GUTZWILLER-TYPE WAVE FUNCTIONS FOR CORRELATED FERMIONS

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In the last few years significant theoretical progress has been made in our understanding of the physics and quality of Gutzwiller-type variational wave functions for correlated Fermi systems. In particular, new analytic techniques are now available that allow for exact evaluations of expectation values. A brief review of the state-of-the-art is presented.

1. Introduction

In view of the tremendous, in general insurmountable, difficulties involved in any exact treatment of interacting quantum mechanical many-body systems, variational wave functions (VWF) are among the very few tools that allow for direct, explicit investigations. Although usually they only yield approximate results, they have the advantage of being physically intuitive and that they can be "custom-tailored" to a particular problem. Furthermore, they can be used even when standard perturbational methods fail or are inapplicable.

VWFs have been extensively used in the investigations of the quantum liquids ^{4}He and ^{3}He.[1] Based on the Jastrow-Feenberg approach a VWF $|\Psi\rangle$ is constructed by letting a correlation operator $\hat{C}$ act on a suitably chosen (simple) one-particle starting wave function $|\phi_0\rangle$ as

$$|\Psi\rangle = \hat{C}|\phi_0\rangle \ . \tag{1}$$

Here $\hat{C}$ describes the microscopic interaction between the particles in some parametrized form. This VWF is then used to calculate expectation values of some operator $\hat{O}$

$$\langle\hat{O}\rangle = \frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \ . \tag{2}$$

In particular, by calculating and minimizing the ground state energy $E_{\mathrm{var}} = \langle\hat{H}\rangle$, where $\hat{H}$ is the Hamiltonian, the variational parameters contained in $\hat{C}$ (and perhaps also in $|\phi_0\rangle$) can be obtained. The variational principle guarantees that E_{var} provides an upper limit for the exact ground state energy.

In principle the same technique can be applied to electronic systems, too.[2] In particular, correlated electrons on a lattice with strong local, i.e. essentially on-site, interactions have always been of great interest. This attention has become even more intense in recent years due to the discovery of heavy fermion systems and high-T_c superconductivity. The simplest, but generic, model for such systems is the Hubbard model[3]

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{I}} , \tag{3}$$

where

$$\hat{H}_{\text{kin}} = \sum_{\mathbf{ij},\sigma} t_{\mathbf{ij}} \hat{c}^{+}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma} , \tag{4a}$$

$$\hat{H}_{\text{I}} = U \sum_{i} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} = U\hat{D} . \tag{4b}$$

Here $\hat{c}^{+}_{\mathbf{i}\sigma}$ ($\hat{c}_{\mathbf{i}\sigma}$) are creation (annihilation) operators of a σ spin ($\sigma = \uparrow,\downarrow$) on site i, with Fourier transforms $\hat{a}^{+}_{\mathbf{k}\sigma}$ ($\hat{a}_{\mathbf{k}\sigma}$) and momentum distribution operator $\hat{n}_{\mathbf{k}\sigma} = \hat{a}^{+}_{\mathbf{k}\sigma} \hat{a}_{\mathbf{k}\sigma}$. The kinetic energy, (4a), is due to quantum mechanical hopping between sites **i** and **j**, which is described by the matrix element $t_{\mathbf{ij}}$, with $\varepsilon_{\mathbf{k}}$ as its Fourier transform. Usually the hopping is restricted to nearest neighbors ("tight binding"), for which $t_{\mathbf{ij}} \equiv -t$. The interaction part, (4b), where $\hat{n}_{\mathbf{i}\sigma} = \hat{c}^{+}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{i}\sigma}$, is purely on-site and thus applies to opposite spins only. Clearly $\hat{D} = \Sigma_{\mathbf{i}} \hat{D}_{\mathbf{i}}$ with $\hat{D}_{\mathbf{i}} = \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow}$ is the number operator for doubly occupied sites in the system.

To obtain an approximation for the ground state energy of (3) Gutzwiller[3] suggested a VWF, $|\Psi_G\rangle$, where the correlation operator in (1) is purely determined by the on-site interaction of the model, (4b), with $|\phi_0\rangle$ as the (noninteracting) Fermi sea $|FS\rangle$

$$|\Psi_G\rangle = g^{\hat{D}} |FS\rangle \tag{5a}$$

$$= \prod_{\mathbf{i}} [1 - (1 - g)\hat{D}_{\mathbf{i}}] |FS\rangle . \tag{5b}$$

Here g is a variational parameter ($0 \leq g \leq 1$). The operator $g^{\hat{D}}$ reduces the amplitude of those spin configurations in $|FS\rangle$ which at a given interaction U contain too many doubly occupied sites. Note that $\hat{D}_{\mathbf{i}} = (1/2)(\hat{n}^2_{\mathbf{i}} - \hat{n}_{\mathbf{i}})$, where $\hat{n}_{\mathbf{i}} = \hat{n}_{\mathbf{i}\uparrow} + \hat{n}_{\mathbf{i}\downarrow}$, such that $\hat{N} = \Sigma_{\mathbf{i}} \hat{n}_{\mathbf{i}}$ is the operator for the total particle number. Hence one may equally well say that $g^{\hat{D}} \sim g^{\Sigma_{\mathbf{i}} \hat{n}^2_{\mathbf{i}}/2}$ suppresses local density fluctuations in a global sense.

In spite of its apparent simplicity analytic evaluations of expectation values of operators, (2), in terms of (5) turned out to be very difficult. There were some perturbational treatments for small U, several numerical evaluations and numerous approximate treatments (for a list of references see Refs. 4, 5). Of

particular importance was the so-called "Gutzwiller approximation" for the ground state energy,[6] which corresponds to a semi-classical counting method of spin configurations.[7] Within this approximation one finds a transition to a localized state at half-filling ($n = 1$), which occurs at a *finite* interaction strength U ("Brinkman-Rice transition"[8]). It leads to simple, "physical" results for a number of problems (metal-insulator transition,[8,9] normal liquid ^{3}He,[4] heavy fermions[10] etc.) and allows one to make contact with well-established theories like Fermi liquid theory ("almost localized Fermi liquid"[4]).

2. Exact, Analytic Evaluations in $d = 1$

Nevertheless, *exact* analytic evaluations of expectation values in terms of (5) for arbitrary interaction strength and band filling were not possible for a long time. Only recently did it become clear that exact evaluations are indeed tractable by a suitable choice of the expansion parameters and the definition of special ("δ-less") contractions, which only involve anticommuting numbers.[5] Noting that $\hat{D}_\mathbf{i} = \hat{n}_{\mathbf{i}\uparrow}\hat{n}_{\mathbf{i}\downarrow}$ is a purely local operator such that the sum $\hat{D} = \Sigma_\mathbf{i}\hat{D}_\mathbf{i}$ involves only *different* sites, expectation values $\langle\hat{O}\rangle$, (2), in terms of (5b) may be written as a sum over different lattice sites only. Thus $\langle\hat{O}\rangle$ takes the form[5]

$$\langle\hat{O}\rangle = \sum_{m=0}^{\infty} \mathcal{O}_m (1 - g^2)^m \,, \tag{6}$$

where $1 - g^2 \leq 1$ is the expansion parameter and the coefficients $\mathcal{O}_m$, which only depend on the density n, can be calculated explicitly by standard field theoretic techniques. These only involve the abovementioned special contractions since all lattice sites are different. The coefficients $\mathcal{O}_m$ correspond to diagrams, whose structure is identical to that of diagrams in any ϕ^4-theory. In this way it is generally possible to calculate *all* orders of $\mathcal{O}_m$ in dimension $d = 1$. In particular, it is possible to evaluate the momentum distribution $\langle\hat{n}_{\mathbf{k}\sigma}\rangle$ — and hence the kinetic energy — as well as the interaction part $\langle\hat{D}\rangle$. After minimization w.r.t. g this yields the variational ground state energy $E(n,U)$ of the Hubbard model, (3).[5] For $n = 1$ and large U the optimized value of g is given by $g = (\overline{U} \ln \overline{U})^{-1}$, such that

$$E = -\left(\frac{4}{\pi}\right)^2 \frac{t^2}{U} \frac{1}{\ln \overline{U}} \,, \tag{7}$$

where $\overline{U} = U/|\overline{\varepsilon_0}|$ with $\overline{\varepsilon_0}$ as the energy of the uncorrelated particles. Hence the exact result for the ground state energy, $\sim -t^2/U$,[10] is here found to be multiplied by a nonanalytic factor $1/\ln \overline{U}$, which increases the energy considerably. For the most part the origin of this additional factor appears to be due to a lack of correlation between empty and doubly occupied sites in the Gutzwiller VWF. — Since the energy of the Hubbard model for $n = 1$ and large, *but finite*, U thus

obtained is obviously not very good, one might be lured into thinking that the Gutzwiller VWF, (5), was not a good wave function even in the limit $U \gg t$, where the Hubbard model transforms (see below) into the antiferromagnetic Heisenberg model

$$H_{\text{Heis}} = J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \ , \tag{8}$$

with $J = 4t^2/U$.[11] However, as will be discussed below, such a suspicion is unwarranted. In fact, for $g = 0$ the Gutzwiller wave function is an excellent wave function for the Heisenberg model in $d = 1$.[12,13]

The analytic approach described above can equally be used to calculate correlation functions

$$C_j^{XY}(n,g) = \frac{1}{L} \sum_i \langle \hat{X}_i \hat{Y}_{i+j} \rangle - \langle \hat{X} \rangle \langle \hat{Y} \rangle \ , \tag{9}$$

for the Hubbard model in terms of $|\Psi_G\rangle$, (5), for arbitrary n and U.[13] Here $\hat{X}_i$, $\hat{Y}_i$ are any one of the four local operators describing the spin ($\hat{S}_i^z = \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}$), the density ($\hat{N}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$), an empty site ($\hat{H}_i = (1 - \hat{n}_{i\uparrow})(1 - \hat{n}_{i\downarrow})$), or a doubly occupied site ($\hat{D}_i$) at site $\mathbf{i}$ (local Cooper pairs with $S = 0$ can also be considered), and $\hat{X} = L^{-1} \Sigma_i \hat{X}_i$ with L as the number of lattice sites. Again exact analytic evaluations are possible in $d = 1$. In particular, the spin-spin correlation function $C_j^{SS}(n,g)$, $j = |\mathbf{j}|$, for $n = 1$ and $U = \infty$ is found as[13]

$$C_{j>0}^{SS}(n = 1, g = 0) = (-1)^j \frac{Si(\pi j)}{\pi j} \tag{10a}$$

$$\sim \frac{(-1)^j}{2j}, \quad j \to \infty \ , \tag{10b}$$

where $Si(x)$ is the sine-integral. The asymptotic behavior implies a logarithmic divergence of $C^{SS}(q)$, the Fourier transform of C_j^{SS}, at half the reciprocal lattice vector, i.e., is of antiferromagnetic origin. Comparison with the exact results for the spin correlation function for the Heisenberg model in the case[14] of $j = 1, 2$ and for large j, where $C_j^{SS} \sim (-1)^j j^{-1} (\ln j)^{1/2}$,[15] show that for $g = 0$ (i.e., $U = \infty$) the Gutzwiller wave function $|\Psi_G\rangle$, (5), yields excellent results in $d = 1$.[13] The same is true for hole-hole correlations in the limit $n \lesssim 1$ and $U = \infty$. Subsequently Haldane, and independently Shastry, recognized that (10a) is, in fact, the exact result for the continuum bose gas in $d = 1$.[16] Thus they proved that $|\Psi_G\rangle$ is the *exact* ground state of a spin 1/2 antiferromagnetic Heisenberg model with an exchange interaction falling off as $1/r^2$.

We may now understand why the Gutzwiller VWF, (5), which does not lead to a good ground state for the half-filled, one-dimensional Hubbard model in the

limit of large, but *finite* U can nevertheless be an excellent wave function for the Heisenberg model. The Heisenberg model involves strictly localized spins; therefore its ground state energy is solely determined by the quality of *spin* correlations. On the other hand, in the Hubbard model for $U<\infty$ there is always a finite amount of hopping, leading to a finite density of doubly occupied sites. Therefore its ground state energy is also determined by *density* correlations. The exact ground state $|\Psi_{ex}\rangle$ of the latter model to order t/U is given by first order degenerate perturbation theory as

$$|\Psi_{ex}\rangle = |\Psi_{Heis}\rangle + \frac{\alpha}{U}\hat{H}_{kin}|\Psi_{Heis}\rangle \ , \tag{11a}$$

where $|\Psi_{Heis}\rangle$ is the exact ground state of the Heisenberg model, α is a numerical constant and $\hat{H}_{kin}$ is given by (4a). Clearly, $|\Psi_{ex}\rangle$ has precisely one doubly occupied site, with one empty site next to it. On the other hand, for $U\to\infty$, i.e. $g\to 0$, the Gutzwiller VWF has the form

$$|\Psi_G(g)\rangle = |\Psi_G(0)\rangle + g_0|\Psi^{(1)}\rangle \tag{11b}$$

where $|\Psi^{(1)}\rangle$ is that contribution to the wave function of the Fermi sea that contains one doubly occupied and an empty site, and $g_0 = [\overline{U}\ln\overline{U}]^{-1}$ is the optimized value of g. The spatial correlation between the doubly occupied and the empty site (described by the second term in (11a) and (11b), respectively) is seen to be strict in the case of (11a), but is quite unspecific, i.e., weak, in the case of (11b). But it is precisely this second term in (11b), i.e. the density correlation, which determines the ground state energy E_{Hub} of the *Hubbard* model at large U. Hence it is the deficiency of density correlations in $|\Psi^{(1)}\rangle$ that is responsible for the logarithmic correction in (7). This deficiency does not enter in $|\Psi_G(0)\rangle$, since the latter does not contain doubly occupied and empty sites anyway.

An assessment of the quality of $|\Psi_G(0)\rangle$ relative to $|\Psi_{Heis}\rangle$ cannot be obtained from the ground state energy E_{Hub} of the Hubbard model, since *both* yield $E_{Hub} = 0$. The quality is only determined by the spin correlations and is known to be excellent[12,13]. This fact may be used to construct a new VWF from the Gutzwiller wave function $|\Psi_G(0)\rangle$[17]

$$|\Psi(\lambda)\rangle = e^{\lambda\hat{H}_{kin}}|\Psi_G(0)\rangle \ , \tag{12a}$$

with $0\leq\lambda\leq\infty$ as a variational parameter. For small λ one has

$$|\Psi(\lambda)\rangle = |\Psi_G(0)\rangle + \lambda\hat{H}_{kin}|\Psi_G(0)\rangle + \mathcal{O}(\lambda^2) \ , \tag{12b}$$

which has the same form as (11a) and yields a very good approximation for E_{Hub} to order t^2/U. Unfortunately it has not been possible so far to calculate with (12a) for arbitrary λ.

3. Exact, Analytic Evaluations in $d = \infty$

Most recently it has been shown by Metzner and Vollhardt[18] that the concept of high spatial dimensions — which in the case of classical as well as localized quantum mechanical spin systems is closely related to the respective mean field theories — is a very helpful approach also for *itinerant* lattice fermions. Provided that the kinetic energy is scaled properly ($t \to t^*/\sqrt{2d}$, with t^* fixed), so that it stays finite in the limit $d \to \infty$, the Hubbard model and the correlations described by it remain non-trivial even in $d = \infty$. For this type of scaling the density of states for a hypercubic lattice in the limit $d = \infty$ becomes

$$N(E) = \frac{1}{\sqrt{2\pi}t^*} e^{-(1/2)(E/t^*)^2} . \tag{13}$$

At the same time diagrammatic treatments become very much simpler than in finite dimensions. This property makes analytic calculations tractable in $d = \infty$, which are prohibitively difficult in lower dimensions. Within a very short time this concept has turned out to be extremely useful in a number of different problems both in variational calculations and Green's function investigations.[19] In the case of generalized, "Gutzwiller-correlated" VWFs of the form

$$|\Psi\rangle = g^{\hat{D}} |\Phi_0\rangle , \tag{14}$$

where $|\Phi_0\rangle$ is now an arbitrary, normalized one-particle product wave function, diagrammatic evaluations of expectation values are greatly simplified in $d = \infty$.[18] The reason for this is easily understood. In analogy to the standard diagrammatic techniques for many-particle systems, the diagrams involved in the evaluation may conveniently be expressed by the self-energy $S_{\sigma,\mathbf{ij}}$ in position space. While vertices in a diagram correspond to a factor $(g^2 - 1)$, the lines in a diagram correspond to the one-particle density matrix for the non-interacting system $P^0_{\sigma,\mathbf{ij}} \equiv \langle \Phi_0 | \hat{c}^+_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} | \Phi_0 \rangle$. In the limit $d \to \infty$ the latter has the property

$$P^0_{\sigma,\mathbf{ij}} \sim \mathcal{O}\left[\left(\frac{1}{\sqrt{d}}\right)^{|\mathbf{i}-\mathbf{j}|}\right] , \tag{15}$$

where $|\mathbf{i} - \mathbf{j}| = \Sigma_{l=1}^{d} |\mathbf{i}_l - \mathbf{j}_l|$. This implies a *collapse* of those diagrams in which two vertices $\mathbf{i}$ and $\mathbf{j}$ are joined by more than two different paths (see Fig. 1). This is the case in particular for the *proper* self energy $S^*_{\sigma,\mathbf{ij}}$, which is the sum over all one-particle irreducible self-energy diagrams. Therefore $S^*_{\sigma,\mathbf{ij}}$ is seen to become *site-diagonal* in $d = \infty$ (see Ref. 18),

$$S^*_{\sigma,\mathbf{ij}} = S^*_{\sigma,\mathbf{ii}} \delta_{\mathbf{ij}} . \tag{16}$$

It should be stressed that these simplifications do not only arise in calculations involving Gutzwiller-correlated VWFs but occur also in *any general Green's*

function approach, where lines correspond to the usual propagators. Defining dressed lines $\bar{P}_\sigma = P_\sigma^0 + P_\sigma^0 S_\sigma P_\sigma^0$, where P_σ^0 and S_σ are considered as matrices in position space, one can introduce skeleton diagrams, which, after collapse, have a very simple "flower structure", that can be summed exactly, yielding

$$S^*_{\sigma,\mathbf{ii}} = -\frac{1}{2\bar{P}_{\sigma,\mathbf{ii}}}\left[1 - \sqrt{1 + 4(1-g^2)\bar{P}_{\sigma,\mathbf{ii}}\bar{P}_{-\sigma,\mathbf{ii}}}\right] . \tag{17}$$

When supplemented by the Dyson equation this expression determines S^*_σ and S_σ for given $|\Phi_0\rangle$ and g.

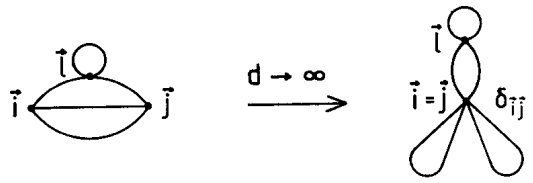

Fig. 1. Collapse in $d = \infty$ of a typical diagram contributing to the proper self-energy $S^*_{\sigma,\mathbf{ij}}$.

The expectation values of the kinetic and the interaction part of the Hubbard Hamiltonian, (3), i.e. of the ground state energy itself, are completely determined by S_σ. Hence, given the starting wave function $|\Phi_0\rangle$ in (14) the evaluation of the ground state energy can be performed explicitly in $d = \infty$. In particular, when $|\Phi_0\rangle$ is given by the Fermi sea $|FS\rangle$, (14) corresponds to the original Gutzwiller VWF, (5). Since the $|FS\rangle$ is translationally invariant, $S^*_{\sigma,\mathbf{ii}}$ does not depend on $\mathbf{i}$, i.e., is simply a global function of g and n, which can be obtained, for example, from particle conservation ($L^{-1}\Sigma_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} = n$). Thereby one obtains

$$S^*_\sigma = \frac{\{A_\sigma - [A_\sigma^2 - 4(1-g^2)(1-n_\sigma)n_{-\sigma}]^{1/2}\}}{2(1-n_\sigma)} , \tag{18}$$

where $A_\sigma = 1 - (1-g^2)(n_\sigma - n_{-\sigma})$. By Dyson's equation the Fourier transform of the self-energy, $S_\sigma(\mathbf{k})$, is then given by $S_\sigma = S^*_\sigma / (1 - S^*_\sigma)$ for $k < k_{F\sigma}$ and $S_\sigma = S^*_\sigma$ for $k > k_{F\sigma}$. The momentum distribution $\langle \hat{n}_{\mathbf{k}\sigma} \rangle$ is therefore a step function with a discontinuity

$$q_\sigma = 1 - \frac{S^*_\sigma}{(1+g)^2}\left(1 - \frac{g^2}{1 - S^*_\sigma}\right) , \tag{19}$$

and the expectation value of the interaction part is given by

$$\langle \hat{D} \rangle = L \frac{g^2 n_\sigma}{1-g^2} \frac{S^*_\sigma}{1 - S^*_\sigma} \tag{20}$$

with $\langle \hat{D} \rangle / L \equiv \mathbf{d}$. Thus the ground state energy E is found as

$$E = L\left(\sum_{\sigma} q_{\sigma} \bar{\varepsilon}_{0\sigma} + \bar{d}\right) . \tag{21}$$

These are precisely the results of the *Gutzwiller approximation.* This semi-classical approximation, which evaluates matrix elements by calculating the *classical* statistical weights of different spin configurations in the non-interacting wave function, and which thereby neglects spatial correlations, is hence seen to yield the *exact* result for the ground state energy in terms of the Gutzwiller VWF in $d = \infty$.[18] As will be described below the above formalism allows for exact evaluations of the Hubbard Hamiltonian and related Hamiltonians in terms of increasingly refined VWF in $d = \infty$.

The diagrammatic method can, of course, also be used to calculate other quantities, such as correlation functions, in terms of Gutzwiller-correlated VWFs, (14). In the case of correlation functions only those diagrams having a bubble-structure of dressed lines remain, i.e., the exact evaluation in $d = \infty$ leads to an overall RPA-type structure.[20] For example, the Fourier transform $C^{SS}(\mathbf{k}; n, g)$ of the spin-spin correlation function $C_{\mathbf{j}}^{SS}(n, g)$, (9), evaluated in terms of the Gutzwiller VWF yields

$$C^{SS}(\mathbf{k}, n, g) = \frac{C^{SS}(\mathbf{k}; n, 1)}{1 - V_s C^{SS}(\mathbf{k}; n, 1)} , \tag{22}$$

where $n/2 = n_{\uparrow} = n_{\downarrow}$, $V_s = (n - 2\bar{d}_0)^{-1} - (n - 2\bar{d})^{-1}$ is a renormalized coupling constant, and $\bar{d}_0 = (n/2)^2$. The transformation into position space is quite intricate; for nearest neighbor positions $\mathbf{j} = \pm \hat{\mathbf{e}}_i$ (and only in this case!) one finds that $C_{\mathbf{j}}^{SS}$ is proportional to its value in the *non-interacting* case ($U = 0$, i.e. $g = 1$).

$$C_{\pm \hat{\mathbf{e}}_i}^{SS} = g_{SS} C_{\pm \hat{\mathbf{e}}_i}^{SS} \big|_{U=0} . \tag{23}$$

Here $g_{SS}(n, g) = [(n - 2\bar{d})/(n - 2\bar{d}_0)]^2$ is a renormalization factor ($1 \leq g_{SS} \leq 4$) describing an enhancement of the spin correlations relative to the non-interacting case. This result had been obtained earlier by Zhang *et al.*[21] via semi-classical counting of spin configurations, i.e., by a Gutzwiller-type approximation. However, this enhancement is merely a *relative* effect, since the *absolute* value of nearest neighbor spin correlation is determined by $(C_{\pm \hat{\mathbf{e}}_i}^{SS}) \big|_{U=0}$ which is of order of the inverse dimension *small*, i.e., vanishes altogether for $d = \infty$.[20] Hence the Gutzwiller VWF, which for $U = \infty$ was found to be excellent in $d = 1$, is inadequate in high dimensions. This is true at least in the case of large U, where the Néel-state, having pronounced nearest neighbor correlation, is known to become the exact ground state.[22] This is also borne out by numerical calculations of the spontaneous magnetization of the Heisenberg model in $d = 2$ which appears to be finite, while (5) yields a vanishing magnetization.[23] Hence in dimensions

$d>1$ and for large U more refined starting wave functions have to be used in (14) to describe the ground state of the Hubbard model (see below). It should be pointed out, however, that Gutzwiller-type approximations are no longer applicable in this case since, in general, they are not systematic.[24]

The exact evaluations of C_j^{SS} in terms of (5) in $d=1$ and $d=\infty$ also shed light on the conditions for the existence of the "Brinkman-Rice transition".[8] This transition, where particles become localized at a *finite* value of U is obtained within the Gutzwiller approximation for the ground state energy, (21).[4] Employing rather general scaling arguments for the asymptotic behavior of C_j^{SS} for $j\to\infty$, one finds that the transition is *absent* in any finite dimension.[20]

4. Application of the Limit $d=\infty$ to Other Gutzwiller-Correlated Wave Functions

The evaluation in terms of VWFs in $d=\infty$ described so far is exact and complete and may in principle be used for an arbitrary starting wave function $|\Phi_0\rangle$ in (14). We mention three examples:

(i)
$$|\Phi_{0,\mathrm{AFHF}}\rangle = \prod_{\mathbf{k},\sigma} [u_{\mathbf{k}}\hat{a}^+_{\mathbf{k}\sigma} + \sigma v_{\mathbf{k}}\hat{a}^+_{\mathbf{k}+\mathbf{Q},\sigma}]\,|0\rangle\ , \tag{24}$$

where $\mathbf{Q}$ is half a reciprocal lattice vector and $|0\rangle$ is the vacuum; (24) is the usual antiferromagnetic Hartree-Fock (AFHF) wave function for the Hubbard model where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ have to be determined variationally.

(ii)
$$|\Phi_{0,\mathrm{PAM}}\rangle = \prod_{\mathbf{k},\sigma} [1 + A(\mathbf{k},\sigma)\hat{f}^+_{\mathbf{k}\sigma}\hat{a}_{\mathbf{k}\sigma}]\,|FS\rangle\ , \tag{25}$$

is used in the case of the periodic Anderson model (PAM),[10,25] and contains a hybridization between f-electrons ($\hat{f}_{\mathbf{k}\sigma}$) and conduction electrons ($\hat{a}_{\mathbf{k}\sigma}$), described by $A(\mathbf{k},\sigma)$;

(iii)
$$|\Phi_{0,\mathrm{BCS}}\rangle = \prod_{\mathbf{k}} [u_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^+_{\mathbf{k}\uparrow}\hat{a}^+_{-\mathbf{k}\downarrow}]\,|0\rangle\ , \tag{26}$$

is the BCS wave function — which when inserted into (14) with the limit $\langle\hat{D}\rangle\to 0$ taken — is a particular representation of the "resonating valence bond" (RVB) wavefunction proposed by Anderson for high T_c superconductivity[26].

In all cases have exact evaluations of the ground state energy of the respective Hamiltonians been shown to be tractable in $d=\infty$.[18,19,24,27,28] In particular, in the case of $|\Phi_{0,\mathrm{AFHF}}\rangle$, (24), the results of the slave-boson saddle-point approximation to a functional integral representation of the Hubbard model[29] are recovered[18,24,27] (for the phase diagram obtained thereby, see Refs. 18, 27, 30). In this way it has been possible to construct the explicit *wave function*, for which

this result is exact (in $d = \infty$). Concerning $|\Phi_{0,\mathrm{PAM}}\rangle$ the results obtained earlier within a Gutzwiller-type approximation[10,31] are recovered.[24,28]

5. The Optimal Form of Gutzwiller-Correlated Wave Functions

Although the formalism for the evaluation of expectation values described above is exact and complete, an explicit evaluation of, say, the proper self-energy $S^*_{\sigma,\mathbf{ii}}$ is still rather involved, or even untractable, when it comes to somewhat more refined starting wave functions $|\Phi_0\rangle$. This has to do with the fact that, in spite of the considerable simplifications arising from the collapse of diagrams in $d = \infty$, a particular subclass of diagrams (that having a "flower-form") still survives in this limit. An ultimate simplification would certainly be achieved if diagrams vanished altogether in $d = \infty$. This can only happen if lines in a diagram vanish identically for equal site indices, i.e., if lines correspond to a one-particle density matrix

$$\tilde{P}^0_{\sigma,\mathbf{ij}} = P^0_{\sigma,\mathbf{ij}} - P^0_{\sigma,\mathbf{ii}}\delta_{\mathbf{ij}} \,, \tag{27}$$

where the site-diagonal part vanishes: $\tilde{P}^0_{\sigma,\mathbf{ii}} = 0$. Such a variant of the diagrammatic formaliksm can indeed be formulated[24], provided the starting wave functions in (14) is written as

$$|\Phi_0\rangle = g^{-\sum_{\mathbf{i},\sigma}\mu_{\mathbf{i},\sigma}\hat{n}_{\mathbf{i}\sigma} + \sum_{\mathbf{i}}\eta_{\mathbf{i}}} |\tilde{\Phi}_0\rangle \tag{28}$$

where $|\tilde{\Phi}_0\rangle$ is again an arbitrary, normalized one-particle product wave function and $\mu_{\mathbf{i},\sigma}$, $\eta_{\mathbf{i}}$ are explicit functions of g and the on-site densities $n^0_{\mathbf{i}\sigma} = \langle\tilde{\Phi}_0|\hat{n}_{\mathbf{i},\sigma}|\tilde{\Phi}_0\rangle$. With this reinterpretation the diagrammatic calculations remain identical to the earlier ones — only the vertices are given a new value and lines now correspond to $\tilde{P}^0_{\sigma,\mathbf{ij}}$. This approach has the great advantage that all results in $d = \infty$ are obtained without the calculation of a single graph, i.e. the VWF based on (28) has the optimal form. In particular, for arbitrary $|\tilde{\Phi}_0\rangle$ (which need not be translationally invariant) one finds a generalization of the result of the Gutzwiller approximation in the case of the translationally invariant VWF, (5),[24]

$$\frac{(1 - n^0_{\mathbf{i}\uparrow} - n^0_{\mathbf{i}\downarrow} + \bar{d}_{\mathbf{i}})\bar{d}_{\mathbf{i}}}{(n^0_{\mathbf{i}\uparrow} - \bar{d}_{\mathbf{i}})(n^0_{\mathbf{i}\downarrow} - \bar{d}_{\mathbf{i}})} = g^2 \,, \tag{29}$$

where $\bar{d}_{\mathbf{i}} = \langle\hat{D}_{\mathbf{i}}\rangle$. This result, which is characteristic for a quasi-chemical approximation, is hence seen to be valid even *locally* in $d = \infty$. Furthermore, the ground state energy for the Hubbard model is obtained as[24]

$$E = \sum_{\langle\mathbf{ij}\rangle} \sqrt{q_{\mathbf{i}\sigma}q_{\mathbf{j}\sigma}}\, P^0_{\sigma,\mathbf{ij}} + U\sum_{\mathbf{i}} \bar{d}_{\mathbf{i}} \,, \tag{30}$$

where now $P^0_{\sigma,ij} = \langle \tilde{\Phi}_0 | \hat{c}^+_{i\sigma}\hat{c}_{j\sigma} | \tilde{\Phi}_0 \rangle$ and $q_{i\sigma}$ is given by (19) under the replacement $n_\sigma \to n^0_{i\sigma}$. For the translationally invariant Gutzwiller VWF, (5), $|\Phi_0\rangle$ and $|\tilde{\Phi}_0\rangle$ are identical up to a trivial factor and $q_{i\sigma} \equiv q_\sigma$; thus (21) is rederived. The general result (30) was first determined by Kotliar and Ruckenstein[29] from a slave boson approach to the Hubbard model. Here we find that in $d = \infty$ the general Gutzwiller-correlated VWFs reproduce the full set of static saddle point equations, thus making the first explicit contact between these two seemingly different approaches. All results for VWFs obtained by the method of Refs. 5, 18 and 27 can easily be derived within the formalism just described.[24]

6. 1/*d* Corrections: Extension to Finite Dimensions

It is natural to extend the above formalism, developed for $d = \infty$, to finite dimensions d by expanding around $d = \infty$. This can be achieved by different methods. They all rest on the principle that in finite dimensions, the collapse of the vertices in a diagram in $d = \infty$ has to be reversed, i.e. the vertices have to be "pulled apart" again. One way is to expand the proper self-energy $S^*_\sigma(\mathbf{k})$ around its value in $d = \infty$, S^*_σ, i.e. to write[27]

$$S^*_\sigma(\mathbf{k}) \approx S^*_\sigma + \sum_{m=1}^{M} [S^*_{\sigma,m}(\mathbf{k}) - S^*_{\sigma,m}] \,, \tag{31}$$

where $S^*_{\sigma,m}$ is the mth-order contribution to S^*_σ (see (6)) and $S_{\sigma,m}{}^*(\mathbf{k})$ is the mth-order contribution to the proper self-energy in d dimensions. Clearly, for $M \to \infty$ (31) approaches the exact d-dimensional result, while for $M = 1$ one recovers the results for the Gutzwiller approximation. By calculating the diagrams for $M = 2,3$ etc. one can easily reproduce the results obtained for the Gutzwiller VWF, (5), by variational Monte Carlo[32] in $d = 2$, 3, e.g. for $\langle \hat{D} \rangle$. Even the exact analytic result for $d = 1$ (see Ref. 5) is well reproduced.

A different avenue to $d < \infty$ is that of an explicit, systematic $1/d$ expansion based on using (28).[24] While in $d = \infty$ all diagrams vanish, the $1/d$ correction in the case of the Gutzwiller VWF requires the calculation of a single diagram; even for the $1/d^2$ correction at $n = 1$ only three diagrams have to be included. Thereby all numerical results (e.g. for $\langle \hat{D} \rangle$ or the kinetic energy of holes) by Yokoyama and Shiba[32,33] obtained with (5) in $d = 2,3$, and even the analytic result in $d = 1$ (see Ref. 5), are very well described by the analytic expansion up to order $1/d$. — It is interesting to note that finite orders of perturbation theory in $1/d$ do *not* remove the Brinkman-Rice transition,[8] which only exists in $d = \infty$.[20,24] Nevertheless as argued earlier,[34] one finds that in $d = 3$ and for $n = 1$ the Gutzwiller approximation is indeed excellent if one is not too close to this transition, i.e. for all $g \geq 0.05$, and is even better for $n < 1$.[24,27]

The analysis of $1/d$ corrections also shows[24] that semi-classical counting arguments, which — as explained above — yield the exact result for the Gutzwiller VWF in $d = \infty$,[5,27] *fail* if $|\Phi_0\rangle$ in (14) has a broken symmetry (e.g. as in (24),

(26)). In particular, simple dependences such as (23), where the correlated quantity is given by the uncorrelated one multiplied by an overall amplification factor, are in general incorrect for several reasons[24]: (i) the correlated quantity is usually the sum of different terms (e.g. the x and z components in the case of the spin correlation function), each of which has its own amplification factor and, (ii) it is not possible to obtain *all* $1/d$ corrections consistently. On the other hand, counting arguments are still applicable in the case of single-particle quantities if $|\Phi_0\rangle$ in (14) is written in the form (28). This is already evident from the fact that the quasi-chemical approximation, which can be obtained by semi-classical counting, is valid in this case (see (29)).

7. Discussion

Gutzwiller variational wave functions and their generalizations have received renewed attention over the last few years, in particular in the context of liquid Helium 3, heavy fermion systems and high T_c superconductors. Analytic techniques permitting exact evaluations of expectation values in terms of these wave function have been developed only recently.[5,18,24] They allow for an unambiguous assessment of the quality of these wave functions. In particular, the limit of high spatial dimensions for correlated lattice fermions[18,19,24,27] has turned out to be very useful: it clarified the validity of the well-known Gutzwiller approximation, revealed intimate connections to slave boson saddle point approximations and, by calculating explicit $1/d$ corrections, is able to make direct connections to finite dimensions, e.g. $d = 2,3$.

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