NEW EXACTLY TRACTABLE LIMITS FOR CORRELATED LATTICE FERMIONS: HIGH DIMENSIONALITY AND INFINITE RANGE HOPPING

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We discuss two different limits where correlated lattice fermions are explicitly tractable: that of infinite range hopping and that of high dimensions. While in the first case results are almost trivial, the latter limit turns out to be particularly significant, since in $d = \infty$ theoretical investigations are enormously simplified, while at the same time correlations remain non-trivial. Contact to finite dimensions can be made via systematic 1/d-expansions. We review the state-of-art of this approach.

INTRODUCTION

Fermions obey the Pauli exclusion principle. Accordingly, their wave function must be antisymmetric. This basic underlying property implies that microscopic investigations of systems with many fermions are faced with a catastrophic "inflation of minus-signs", which leads to immense, in general untractable, technical problems. Indeed, the antisymmetry requirements lead to substantial spatial correlations even in a Fermi gas. Interactions, particularly those of short range, then introduce additional subtle phase relations. Although these problems are known for a long time, they have received a wide attention only in recent years in the context of strongly correlated Fermi systems such as heavy fermions and high-T_c superconductivity.

Of all analytic methods for the investigation of the ground state of interacting Fermi systems, the Bethe-ansatz is the most successful. Unfortunately, this approach only works for some particular quantum mechanical models in d = 1 dimensions. By contrast, standard many-body perturbation techniques can be applied in all dimensions; in practice, however, they are limited to certain parameter ranges, e.g. very weak or very strong interactions, low densities etc. At the same time mean field theories, slave boson approaches or variational methods are more easily tractable and often provide valuable insight; nevertheless their actual validity is usually hard to estimate. While these problems apply to all Fermi systems, they are most severe in the case of systems with itinerant degrees of freedom as in the Hubbard model, because one then has to work explicitly with fermion operators. The case of localized degrees of freedom, where the spins have a fixed position as in the Heisenberg model, is - relatively speaking - considerably simpler, since this only involves spin operators. In the present paper we will mainly address the former case, i.e. itinerant spin systems.

In view of the theoretical difficulties mentioned above it is of considerable help if one is at least able to obtain exact results for a model in certain extreme limits of the parameters of the model. If a solution is possible at all, it often turns out that perturbation techniques etc. are able to connect this solution to more realistic parameter values.

THE HUBBARD MODEL AS A GENERIC MODEL

The Hubbard model[1] combines the kinetic energy of electrons, i.e. band behavior, with a highly simplified description of the (strongly screened) Coulomb interaction between up/down spins on a lattice. Its Hamiltonian is given by

$$H = H_0 + H_I \tag{1a}$$

where

$$H_0 = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} = \sum_{k,\sigma} \varepsilon_k a^{\dagger}_{k\sigma} a_{k\sigma} \tag{1b}$$

$$H_I = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = U \sum_k \hat{\rho}_{k\uparrow} \hat{\rho}_{-k\downarrow} \tag{1c}$$

Here $c^{\dagger}_{i\sigma}(c_{i\sigma})$ are creation (annihilation) operators of a σ-spin ($\sigma = \uparrow,\downarrow$) on site i, whose Fourier transforms are $a^{\dagger}_{k\sigma}(a_{k\sigma})$. The kinetic energy H_0, (1b), is due to quantum mechanical hopping between sites i and j, which is described by the matrix element t_{ij}, whose Fourier transform is the energy dispersion ε_k. Usually hopping is considered to occur only between nearest neighbors ("tight binding"). The interaction H_I, where $\hat{n}_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$, only acts on the same site and only for opposite spins; hence $\hat{D}_i = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ is the operator for double occupancy. This particular interaction is an essential part of many model Hamiltonians. In (1c) $\hat{\rho}_{k\sigma}$ is the electron density operator

$$\hat{\rho}_{k\sigma} = \frac{1}{\sqrt{L}} \sum_q a^{\dagger}_{q\sigma} a_{q+k\sigma} \tag{2}$$

At U = 0 one has a free gas of lattice electrons, while at U=∞ the spins are localized. In fact, in the limit ($U \to \infty$) and for $n_{\uparrow} = n_{\downarrow} = n/2$ (half filling) the Hubbard model for nearest neighbor hopping transforms into the antiferromagnetic Heisenberg model

$$H_{Heis} = \frac{4t^2}{U} \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j \tag{3}$$

In spite of almost three decades of work on the Hubbard model, only very few exact results for the thermodynamic limit are known (for reviews see, for example, refs. 2,3,4). Of these the exact solution in d = 1 for the ground state by Lieb and Wu[5] is the most important. It should be noted that even the mean field theory for the Hubbard model is non-trivial and cannot be solved in generality.

LIMIT OF INFINITE RANGE HOPPING ($t_{ij} = -t$)

The Hubbard model, (1), can be solved exactly if the zero-range interaction, (1c), is replaced by an interaction of infinite range. In this case one obtains a trivial mean field model, whose wave function is simply that of the noninteracting Fermi sea (naive Hartree-Fock).

A much less obvious limit is that where the quantum mechanical hopping of the electrons is assumed to be unconstrained, i.e. is taken as infinite ranged ($t_{ij} \equiv -t$ for all $i \neq j$). In this situation the model clearly no longer depends on the dimension or the lattice structure. The energy dispersion is then given by

$$\varepsilon_k = -tL\ \delta_{k,0} \tag{4}$$

where L is the number of lattice sites. The model takes the form

$$H = -tL \sum_{\sigma} \hat{n}_{k=0,\sigma} + U \sum_{k} \hat{\rho}_{k\uparrow}\ \hat{\rho}_{-k\downarrow} - \mu \sum_{k,\sigma} \hat{n}_{k\sigma} \tag{5}$$

where we included a chemical potential for generality. It should be noted that the kinetic remains extensive, i.e. scaling with L is not required. (This is a consequence of the fact that the operator $a_{k=0,\sigma} = L^{-1/2}\Sigma_i c_{i\sigma}$ still obeys Fermi statistics). Hence the two electrons with $k = 0$ carry the complete kinetic energy of the system. -

The Hubbard model for infinite range hopping, (4), has recently been solved exactly for all temperatures by van Dongen and Vollhardt[6] using standard methods of many-body theory. In essence the solution is made possible by the fact that the momentum state $k = 0$, which rules the kinetic energy, does not play a preferred role in the interaction term, i.e. is only one of the O(L) many states and may therefore be neglected. Consequently, the two parts of the Hamiltonian (4) commute and may be diagonalized separately. The partition

function can then be found exactly for all temperatures T. This yields the exact grand canonical potential as[6]

$$\Omega = L \left[-2t - \beta^{-1} \ln (1 + 2z + z^2 e^{-\beta U}) \right] \tag{6}$$

where $\beta^{-1} = k_B T$ and $z = e^{\beta\mu}$ is the fugacity. In particular, the expectation value of the interaction term, $\langle H_I \rangle = LU\bar{d}$, where $\bar{d}(U,T)$ is the density of doubly occupied sites, is determined by the equation

$$\frac{\bar{d}(1-n_\uparrow-n_\downarrow+\bar{d})}{(n_\uparrow-\bar{d})(n_\downarrow-\bar{d})} = e^{-\beta U} \tag{7}$$

which for $n_\uparrow = n_\downarrow = \frac{1}{2}$ reduces to $\bar{d} = \frac{1}{2}(1 + e^{\beta U/2})^{-1}$. The general result, (7), is seen to have the form of the law of mass action, which determines the equilibrium state of a reversible chemical reaction of the type

$$D + E \longleftrightarrow S_\uparrow + S_\downarrow \tag{8}$$

On the left hand side of the reaction, D (denoting the doubly occupied sites) has a concentration $\bar{d}$ and E (denoting the empty sites) has a concentration $1 - n_\uparrow - n_\downarrow + \bar{d}$; D and E may "react" to form two singly occupied sites $S_\uparrow$, $S_\downarrow$ of opposite spin and with a concentration $(n_\uparrow - \bar{d})$ and $(n_\downarrow - \bar{d})$, respectively. The equilibrium is determined by the Boltzmann factor $e^{-\beta U}$. The form of (7) is typical for a result obtained within the "quasi-chemical approximation" in the theory of mixtures. The fact that this approximation yields the exact result for the model under consideration is not surprising. In the model with infinite range hopping every site can be reached without obstruction due to other sites, thus leading to a perfectly homogeneous "mixture" of site occupations at arbitrary interactions and temperatures. Thus the assumption underlying the quasi-chemical approximation becomes exact here. - It is interesting to note that (7) is also obtained within the wellknown Gutzwiller approximation[7] to the conventional Hubbard model, if $e^{-\beta U}$ is replaced by g^2, where g is a variational parameter entering the trial wave function in this

approach. As will be discussed below the latter approximation is exact in the limit of infinite dimension.[8]

The ground state of the model with unconstrained hopping is somewhat pathological. One finds $\bar{d}(U) = 0$ for $n \leq 1$ and $\bar{d}(U) = n-1$ for $2 \geq n \geq 1$, i.e. the system has a ground state with the least possible number of doubly occupied sites, irrespective of the strength of the interaction. Therefore $\bar{d}(U)$ has a kink at $n = 1$. On the other hand, for $T > 0$ the U-dependence of $\bar{d}$ is precisely what one expects from the conventional Hubbard model, i.e. $\bar{d}(0) = n_\uparrow n_\downarrow$ and an exponential decrease for $U \to \infty$.[6]

The kink in $\bar{d}(U)$ at $n = 1$ implies that in the ground state there occurs a metal-insulator transition at this density for all $U > 0$, i.e. at $n = 1$ the ground state is always insulating but is conducting otherwise.[6] It is remarkable that a model, which in view of $[H_{kin}, H_I] = 0$ is essentially trivial, is nevertheless able to describe a transition which is known to occur also in the exact ground state of the ordinary Hubbard model in $d = 1$ [5] (and most probably also in $d > 1$ in the case of bipartite lattices). The origin of the transition is, of course, quite different in the two cases, being the conse- quence of antiferromagnetic correlations in the latter case.

LIMIT OF INFINITE DIMENSIONS ($d = \infty$)

In classical statistical physics the limit of infinite spatial dimensions is well established, since it often allows for exact solutions. This is due to the fact that for $d \to \infty$ the number of nearest neighbors grows proportional to d, thus making fluctuations unimportant. As a consequence there is an intimate connection between solutions in $d = \infty$ and mean-field-type solution. The same is basically true for quantum mechanical systems of localized spins. For example, in $d = \infty$ the Neél-state becomes the exact ground state of the Heisenberg model.[9]

The question then arises how interacting, itinerant Fermi systems - such as the Hubbard model - behave, and whether they become simple, or even trivial, in $d = \infty$. Until most recently there existed virtually no results for such models in this limit. In this situation one may in particular ask whether mean field solutions (e.g. unrestricted Hartree-Fock) become exact in $d = \infty$.

With these questions in mind Metzner and Vollhardt[8] recently introduced the concept of infinite dimensions for itinerant lattice fermion systems. They showed that, provided the kinetic energy is scaled properly, correlations remain non-trivial even in the limit $d = \infty$. In particular, it was found that diagrammatic treatments become very much simpler than in finite dimensions. This property makes exact analytic calculations tractable in $d = \infty$, which are prohibitively difficult in lower dimensions. Indeed, within a very shortwhile the limit of high dimensions for lattice fermions has proved its usefulness in a number of different problems. In the following we will review the main features of this approach and will at least outline the results obtained within the last nine months by the author's group and various other researchers.

The energy dispersion ε_k for nearest neighbor hopping on a d-dimensional hypercubic lattice, which enters the kinetic energy operator, (1b), has the form

$$\varepsilon_k = \frac{-t}{L} \sum_{<ij>} e^{ik(R_i - R_j)} \tag{9a}$$

$$= -2t \sum_{i=1}^{d} \cos k_i \tag{9b}$$

From (9) one might naively expect that for $d \to \infty$ ε_k was typically of the order of td, such that ε_k had to be scaled with 1/d to obtain a finite kinetic energy. However, this is wrong. For a randomly chosen vector k (9b) yields $\varepsilon_k \sim -t\sqrt{d}$. Indeed,

from the central limit theorem one finds for the density of states (DOS) in the limit $d \to \infty$

$$N(E) = \frac{1}{2t\sqrt{\pi d}} \exp -\left[\frac{E}{2t\sqrt{d}}\right]^2 \tag{10}$$

This clearly shows that only the scaling $t \to t/\sqrt{2d}$, such that $N(E) \to N^*(E) = \exp(-E^2/2t^2)/\sqrt{2\pi}t$, leads to a finite kinetic energy and thereby to a non-trivial quantum mechanical model, (1), where both the kinetic energy and the interaction energy are of the same order of magnitude. With the naive scaling $t \to t/2d$ the kinetic energy would vanish for $d \to \infty$ and one would obtain a trivial model of localized spins. We will now discuss several applications of the concept of high dimensions.

Weak Coupling Correlation Energy

The correlation energy E_c is defined as the difference between the exact energy E and the naive Hartree-Fock energy E_{HF}

$$E_c = E_{exact} - E_{HF} \tag{11}$$

In the case of the Hubbard model $E_{HF} = \bar{\varepsilon}_0 + U n_\uparrow n_\downarrow$, where $\bar{\varepsilon}_0$ is the energy of the non-interacting particles. As shown by Metzner and Vollhardt[10] the result for E_c in weak coupling ($U \to 0$) can be calculated within ordinary Goldstone perturbation theory in any dimension d. The lowest order contribution to E_c in U is given by

$$E_2 = \frac{LU^2}{(2\pi)^{4d}} \sum_f \int \left[\prod_{i=1}^{4} d^d k_i\right] \frac{n_1^0 n_2^0 (1-n_3^0)(1-n_4^0)}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4} e^{i(k_1+k_2+k_3+k_4)f} \tag{12}$$

where $\varepsilon_i \equiv \varepsilon_{k_i}$ and $n_i^0 = 1$ for $\varepsilon_i < E_F$ and zero elsewhere. The sum on the Fourier factor over all lattice sites f is

equivalent to a δ-function, which guarantees conservation of crystal momentum at the vertices, i.e. $\Sigma_i \mathbf{k}_i = 0$. One can now show[8] that in $d = \infty$ only the term with $\mathbf{f} = 0$ gives a finite contribution to (12), and that nearest neighbor contributions etc. only contribute terms of order $1/d$ or smaller. This has the following reason: at a vertex $\Gamma_{kk'}(q)$, where two momenta $\mathbf{k}_\pm = \mathbf{k} \pm \mathbf{q}/2$ enter and two momenta $\mathbf{k}'_\pm$ leave, the momenta $\mathbf{k}$, $\mathbf{k}'$, $\mathbf{q}$ may be chosen arbitrarily; now, in $d = \infty$ the corresponding energies ε_k etc. are randomized by Umklapp-processes, which are generated when the lattice momenta, having infinite number of components, are added. In this situation the energies are no longer related to the initial momenta - they become mutually independent. Equivalently, one may say that in $d = \infty$ momentum conservation at the vertex becomes unimportant, such that $(2\pi)^d \delta(\mathbf{k}) = \Sigma_f e^{i\mathbf{k}\mathbf{f}}$ can be replaced by 1. Clearly, this is identical to setting $\mathbf{f} = 0$ in the sum. (For a more general discussion of this point, see Müller-Hartmann[11]) The integrand in (12) now depends on the momenta $\mathbf{k}_i$ only via the energies ε_i. Using the DOS (10) one can therefore replace the momentum integrations by energy integrations and obtains[8] for $n_\uparrow = n_\downarrow = n/2$

$$E_2/LU^2 = -\int_0^\infty d\lambda\, e^{2\lambda^2} P^2(E_F - \lambda) P^2(-E_F - \lambda) \qquad (13)$$

where $P(x)$ is the probability function. Hence in $d = \infty$ the expression for E_2 is found to have the simplest structure of all dimensions. - It is interesting to note that E_2, (12), had been obtained before by Kajzar and Friedel[12] who evaluated this expression in $d = 3$ by introducing a single site approximation, where only the term with $\mathbf{f} = 0$ was considered in the lattice sum. This "local approximation" has since become a standard approximation scheme in metal physics.[13), 14)] Here we have found that this approximation is exact in the limit $d \to \infty$. In fig. 1 E_2 is shown as a function of density n in dimensions $d = 1, 2, 3, \infty$.[8), 15)] Clearly, the result for $d = 3$, which can only be calculated by considerable numerical effort, is very well approximated by that for $d = \infty$, which is given by

the single integral in (13). In fact, for $n \lesssim 0.8$ even the result for $d = 2$ is well represented by that for $d = \infty$ (the deviation for $n \lesssim 1$ is due to the logarithmic divergence of the DOS for $n = 1$). The fact that $E_2 \propto U^2$ even in $d = \infty$, shows that unrestricted Hartree-Fock theory cannot be exact in $d = \infty$. This mean field theory leads to a non-analytic dependence even of the leading contribution to E_c on U for small U.

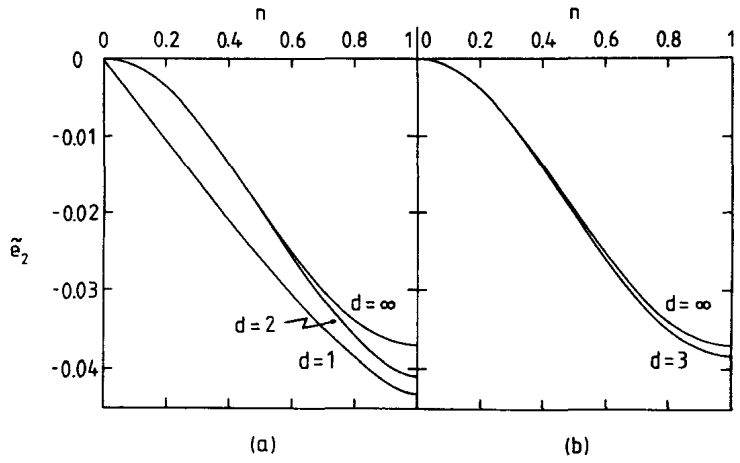


Fig. 1 Lowest order contribution in U to the correlation energy for the Hubbard model $E_2 = L\ \tilde{e}_2(U/2t)^2\ N^*(E_F)$, as a function of the density n for several dimensions d.

Variational Wave Functions

Variational wave functions (VWF) play an important role in the investigations of interacting many body systems, and of strong correlated Fermi systems in particular.[4] They provide an approximate, but explicit and physically intuitive tool for the treatment of correlations and quite generally go beyond the range of perturbation theory.

In the case of spin models with strong on-site repulsion, (1c), the suppression of doubly occupied sites is of prime importance. This suppression is achieved by a wave function of the form

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

$$= \prod_i [1-(1-g)\, \hat{D}_i \,] \, |\Phi_0\rangle \tag{14b}$$

where $\Sigma_i \hat{D}_i = \hat{D}$ is the number operator for doubly occupied sites, $0 \leq g \leq 1$ is a variational parameter and $|\Phi_0\rangle$ is an arbitrary one-particle wave function. The projector $g^{\hat{D}}$ reduces the amplitude of those spin configurations in $|\Phi_0\rangle$ with too many doubly occupied sites. With $|\Phi_0\rangle$ as the simple Fermi sea, (14) reduces to the Gutzwiller wave function (GWF).[1] In spite of the formal simplicity of this wave function, evaluations of expectation values $\langle\hat{O}\rangle = \langle\Psi|\hat{O}|\Psi\rangle/\langle\Psi|\Psi\rangle$ in terms of $|\Psi\rangle$ are not at all simple and had not been possible for a long time. However, recently a new analytic, diagrammatic approach has been formulated, which allows one to evaluate the ground state energy of the Hubbard model in terms of the GWF <u>exactly</u> in $d = 1$.[16] The calculation of correlation functions then showed that the GWF is indeed an excellent wave function for this model in $d = 1$.[17] In fact, for $g = 0$ the GWF is the exact wave function for an $S = \frac{1}{2}$ antiferromagnetic Heisenberg model with $1/r^2$ interaction.[18]

Using standard field-theoretical methods expectation values $\langle\hat{O}\rangle$ can be written in this approach[16] as a power series in (g^2-1) whose coefficients correspond to diagrams. The structure of these diagrams is identical to that for propagators in a ϕ^4-theory.[16],[17] Diagrams are conveniently expressed by the *self-energy* $S_{\sigma f h}$ in position space, with lines corresponding to $P^0_{\sigma f h} = \langle\Phi_0|c^\dagger_{f\sigma} c_{h\sigma}|\Phi_0\rangle$ and vertices corresponding to a factor (g^2-1). Both the one-particle density matrix $P_{\sigma f h} \equiv \langle c^\dagger_{f\sigma} c_{h\sigma}\rangle$, which yields the kinetic energy $\langle H_0\rangle$, (1b), and the on-site interaction $\langle H_I\rangle$, (1c), are completely determined

by $S_{\sigma fh}$.[8),19)]

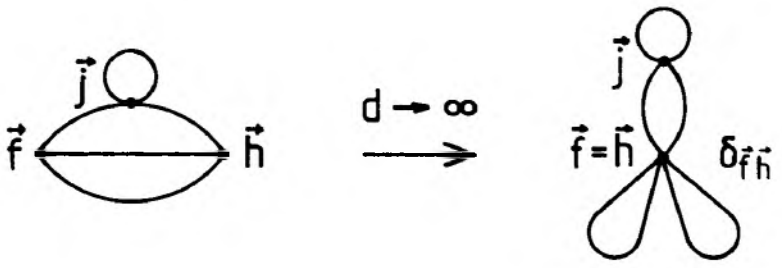
As in the case of the correlation energy, the evaluation of the diagrams for S_σ is tremendously simplified in $d = \infty$.[8),19)] This is due to the fact that $P^0_{\sigma fh}$ vanishes at least as $1/\sqrt{d}$ for $d \to \infty$ if $f \neq h$. As a consequence, those diagrams in which two vertices f, h are connected by more than two separate paths <u>collapse</u>, as shown in Fig. 2. Now, in the proper self-energy $S^*_{\sigma fh}$, which is the sum over all one-particle irreducible self-energy diagrams, all external vertices are always connected by three separate paths. Therefore $S^*_{\sigma fh}$ is seen to become <u>site-diagonal</u> in $d = \infty$

$$S^*_{\sigma fh} = S^*_{\sigma ff}\,\delta_{fh} \tag{15}$$

Introducing skeleton diagrams by defining dressed lines $\bar{P}_\sigma = P^0_\sigma + P^0_\sigma S_\sigma P^0_\sigma$, where P^0_σ and S_σ are taken as matrices, the collapsed skeleton diagrams are found to have a very simple "flower"-structure, which can be summed exactly. This yields

$$S^*_{\sigma ff} = -\frac{1}{2\,\bar{P}_{\sigma ff}}\left[1 - \sqrt{1+4(1-g^2)\bar{P}_{\sigma ff}\bar{P}_{-\sigma ff}}\;\right] \tag{16}$$

which, together with the Dyson equation, determines S^*_σ and S_σ for given P^0_σ and g.



<u>Fig. 2</u> Collaps of a typical self-energy diagram in $d = \infty$.

Ground State Energies

Given the starting wave function $|\Phi_0\rangle$ in (14), the evaluation of, say, the ground state energy of (1) can be performed explicitly in $d = \infty$. We mention three examples.

(i) $|\Phi_0\rangle$ is chosen as the Fermi sea, $|\Phi_0\rangle = |FS\rangle$. Then $|\Psi\rangle$ corresponds to the GWF.[1),7)] Because of translational invariance of $|\Phi_0\rangle$, $S^*_{\sigma f}$ is independent of f, i.e. $S^*_{\sigma f} = S^*_\sigma$ for all f. Thus the problem reduces to calculating the number S^*_σ. The results obtained thereby are precisely those provided by the Gutzwiller approximation[7)], which corresponds to a (semi)-classical counting method of spin configurations. This shows that the results of this approximation for $\langle H\rangle$, (1), in terms of the GWF become exact in $d = \infty$. [8),16),19)]

(ii) To take into account the antiferromagnetic tendencies of the Hubbard-model for $n = 1$, $|\Phi_0\rangle$ may be chosen as the unrestricted Hartree-Fock wave function

$$|\Phi_0\rangle = \prod_{k,\sigma} \left[\cos\theta_k a^+_{k\sigma} + \sigma \sin\theta_k a^+_{k+Q,\sigma}\right] |0\rangle \qquad (17)$$

where the function θ_k has to be determined variationally, $Q = (\pi,\ldots,\pi)$ is half a reciprocal lattice vector and $|0\rangle$ is the vacuum. The ground state energy $E\{g,\theta_k\} = \langle H\rangle$, which is a functional of g and θ_k , can be calculated and minimized in closed form.[8),19)] One finds that the optimal θ_k is in general more complicated than the Hartree-Fock form often used for simplicity in numerical calculations.[20)] The ground state energy is identical to that calculated by Kotliar and Ruckenstein,[21)] who used a slave boson approximation. The results of Ref. 8 and 19 now provide the explicit wave function ((14) with (17)) for which the slave boson result is exact in $d = \infty$. They also yield the magnetization phase diagram as a function of interaction U and particle density. The wave function considered here combines the virtues of the GWF (U^2-dependence of the correlation energy for small U) with the exact antiferromagnetic behavior of (18) at large U.

(iii) The periodic Anderson model (PAM) involves almost localized f-electrons ($f_{k\sigma}$) on a periodic lattice in a sea of conduction electrons ($a_{k\sigma}$), which may hybridize with the f's. A wave function of type (14) with $g \to 0$ has been suggested for this investigation,[22] where

$$|\Phi_0\rangle = \prod_{k,\sigma} \left[1+A_\sigma(k) f^\dagger_{k\sigma} a_{k\sigma}\right] |cFS\rangle \qquad (18)$$

Here $A_\sigma(k)$ describes the hybridization and $|cFS\rangle$ is the Fermi sea of the conduction electrons. As shown by Gebhard and the author [23] the ground state energy of the PAM in terms of (14) with (18) can be evaluated exactly in $d = \infty$. The results agree in detail with those obtained earlier by semi-classical counting arguments à la Gutzwiller,[22),24),25] and those of a slave boson approach.[21]

Correlation Functions

The diagrammatic methods discussed above have been used by van Dongen, Gebhard and the author[26] to calculate correlation functions for Hubbard-type models in terms of projected wave functions. Again the explicit calculation becomes especially simple in $d = \infty$. In this limit only diagrams with bubble-structure remain, such that correlation functions acquire an overall RPA-type form. For example, using the GWF the spin-spin correlation function $C^{ss}_j(n,g) = L^{-1}\Sigma_i \langle S^z_i S^z_{i+j}\rangle - (L^{-1}\Sigma_i \langle S^z_i\rangle)^2$, with $S^z_i = n_{i\uparrow} - n_{i\downarrow}$, can be evaluated in closed form; its Fourier transform is given by

$$C^{ss}(k;n,g) = \frac{C^{ss}(k;n,1)}{1-V_s\, C^{ss}(k;n,1)} \qquad (19)$$

with V_s as a renormalized coupling constant, $V_s = (n-2\bar{d}_0)^{-1} - (n-2\bar{d})^{-1}$, and $\bar{d} = \langle\hat{D}\rangle/L$, $\bar{d}_0 = n_\uparrow n_\downarrow$. The transformation into position space is quite delicate; for next neighbor (n.n.) positions $j = \pm\hat{e}$ one finds that C^{ss}_j is <u>proportional</u> to its value in the noninteracting case ($g = 1$)

$$C^{ss}_{\pm\hat{e}_i}(n,g) = g_{ss}\, C^{ss}_{\pm\hat{e}_i}(n,1) \qquad (20)$$

Here $g_{ss}(n,g) = [(n-2\bar{d})/(n-2\bar{d}_0)]^2$ is a renormalization factor describing an enhancement of the spin correlations relative to the non-interacting case. This result had been obtained earlier by Zhang et al.[27] using semi-classical counting arguments in the spirit of the Gutzwiller approximation.[7] Note, that (20) only holds for n.n. positions. It must be stressed that the enhancement discussed above is only a relative effect. In fact, n.n. spin correlations are only of the order of the inverse dimension, i.e. vanish for $d \to \infty$. [26] Hence the GWF, which is excellent in $d = 1$, is clearly inadequate in high dimensions, since for $U \to \infty$ the Néel-state is known to become the exact ground state.[9] More refined starting wave functions $|\Phi_0\rangle$, such as (17), have to be used in this case. It should be pointed out, however, that counting methods are then generally no longer applicable (see below).

Using the exact results for C^{ss}_j in terms of the GWF in $d = 1$ and $d = \infty$, and employing rather general scaling arguments, one can show[26] that the Brinkman-Rice transition,[28] i.e. the localization of particles at finite U which is obtained within the Gutzwiller approximation[7], is absent in any finite dimension.

The formalism described above is exact and complete and may be used for arbitrary $|\Phi_0\rangle$. Nevertheless, an explicit evaluation of the proper self-energy $S^*_{\sigma ff'}(15)$, is still rather involved when it comes to somewhat more refined wave functions $|\Phi_0\rangle$. To overcome these difficulties Gebhard[29] has worked out a particularly economic method for the calculation of expectation values in terms of variational wave functions in $d = \infty$. He realized that calculations in $d = \infty$ would become even simpler if diagrams not only collapsed, but vanished altogether in this limit. This would be the case if lines in the diagrams corresponded to a one-particle density matrix $\tilde{P}^0_{\sigma fh} = \langle\tilde{\Phi}_0|c^\dagger_{f\sigma}c_{h\sigma}|\tilde{\Phi}_0\rangle$, with $\tilde{P}^0_{\sigma ff} = 0$. The latter property can in-

deed be fulfilled if the arbitrary, normalized one-particle wave function $|\tilde{\Phi}_0\rangle$ is chosen as (see (14))

$$|\Phi_0\rangle = g^{-\sum_{i,\sigma} \mu_{i\sigma} \hat{n}_{i\sigma} + \sum_i \eta_i} |\tilde{\Phi}_0\rangle \tag{21}$$

where $\mu_{i\sigma}$, η_i are explicit functions of $\tilde{n}^0_{i,\sigma} \equiv \langle\tilde{\Phi}_0|\hat{n}_{i\sigma}|\tilde{\Phi}_0\rangle$ and g. The diagrammatic calculations are identical to those in ref. 8,19 but the vertices are given by a new value and lines now correspond to $\tilde{P}^0_{\sigma\, f\, k}$. This approach has the considerable advantage that results in d = ∞ are obtained without having to calculate a single graph. In particular, for arbitrary $|\tilde{\Phi}_0\rangle$ one finds a generalization of the result of the quasi-chemical approximation (7)

$$\frac{\bar{d}_i\,(1-\tilde{n}^0_{i\uparrow}-\tilde{n}^0_{i\downarrow}+\bar{d}_i)}{(\tilde{n}^0_{i\uparrow}-\bar{d}_i)(\tilde{n}^0_{i\downarrow}-\bar{d}_i)} = g^2 \tag{22}$$

which is seen to be valid even <u>locally</u>. The result of the Gutzwiller approximation[7] for the translationally invariant GWF is a special case of (19). - All results for VWFs discussed by the method of ref. 8,19 can also easily be derived within the formalism of ref. 29. Based on his exact optimization of VWFs in d = ∞, Gebhard[29] has proposed explicit, but simple VWFs for the Hubbard, the t-J model[27] and the Heisenberg model which can be used for numerical calculations (variational Monte-Carlo) in finite dimensions and which are expected to yield very good results for the ground state energy.

RESULTS FOR FINITE DIMENSIONS BY (1/d)-EXPANSION

It is natural to extend the above formalism, developed for d = ∞, to finite dimensions by expanding around d = ∞. This can be achieved by different methods. For example, in the case of the GWF Metzner[19] expanded the proper self energy $S^*_\sigma(\mathbf{k})$ around its value in d = ∞, S^*_σ. Thereby one can easily reproduce the results obtained for the GWF by variational Monte Carlo in d = 2,3, e.g. for $\langle\hat{D}\rangle$.[30] Even the exact result

for
$d = 1$ is well reproduced. This also shows that in $d = 3$ and for $n = 1$ the Gutzwiller approximation is indeed excellent for all $g \gtrsim 0.05$ (at $g = 0$ there occurs the localization transition[28]), and that it is even better for $n < 1$.

A different avenue to $d < \infty$ is that of a direct 1/d-expansion [26] as worked out systematically by Gebhard.[29] He finds that all numerical results[20),30)] obtained with the GWF in $d = 2,3$, and even in $d = 1$, (e.g. for $\langle \hat{D} \rangle$ or the kinetic energy of holes) 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 <u>not</u> remove the Brinkman-Rice transition, which should only exist in $d = \infty$.[26),29)]

The analysis of 1/d corrections also shows that semi-classical counting arguments, which - as explained above - yield the exact result for the GWF in $d = \infty$,[8),19)] <u>fail</u> if $|\Phi_0\rangle$ in (14) has a broken symmetry (e.g. as in (18) or in the case of a BCS wave function). In particular, simple dependences such as (20), where the correlated quantity is given by the uncorrelated one multiplied by an amplification factor, are in general incorrect for several reasons:
(i) the correlated quantity is usually the sum of different terms each of which has its own amplification factor and, (ii) the 1/d dependence cannot be obtained consistently.[29] 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 (21). 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 (22)).

THE USE OF GREEN'S FUNCTIONS IN $d = \infty$

Immediately after the $d = \infty$ limit for correlated lattice fermions had been introduced by Metzner and the author,[8)] it

became clear that the limit of high dimensions leads to considerable simplifications also for other models and theoretical approaches. Müller-Hartmann[11] observed that the irrelevance of momentum conservation in those Feynman diagrams, where the number of internal lines is greater than twice the number of relevant vertices, has far-reaching implications for a general Green's function approach. For example, the self-energy becomes momentum-independent in $d = \infty$ (see (15)). Not only is Fermi liquid theory therefore obeyed in $d = \infty$, it is much simpler than even for an isotropic system in $d = 3$. Furthermore, interactions between particles on dif- ferent sites were found to simplify to their Hartree substitute. He then formulated a self-consistent weak coupling theory which could easily be solved numerically.[31] The results show all Fermi liquid features of a correlated Fermi system.

Similarly, Schweitzer and Czycholl[32] investigated the periodic Anderson model within a self-consistent perturbation theory in the on-site Coulomb correlation between the f-electrons in $d = \infty$. Such an investigation had not been feasible before, not even in $d = 1$, since this requires an enormous numerical effort in finite dimensions. The simplification arising in $d = \infty$ reduced these difficulties by several orders of magnitude. At the same time the essential physical behavior (Fermi liquid properties, sum rules, f-electron self-enegy etc.) was found to be essentially the same as in finite dimensions.[32]

The simplifying features arising in $d = \infty$ also made possible the exact solution of the Falikov-Kimball model (a Hubbard model where only one of the two spin-species can move). Making explicit use of the DOS, (10), and of the fact that in $d = \infty$ the proper self-energy Σ_{fh} becomes site-diagonal, as expressed by (15) and discussed in refs. 11,31,32, Brandt and Mielsch[33] showed that Σ_{ff} can be expressed by the site-diagonal Green's function. To obtain Σ_{ff} it is then sufficient to solve the atomic problem in a generalized time-dependent external field. This they were able to do and thereby they

obtained the temperature dependence of the equilibrium Green's function and of several correlation functions for this model in $d = \infty$ and $T > T_c$.

Finally, Metzner[34] explicitly calculated the Green's function for the Hubbard model in $d = \infty$ at $n = 1$ and $T = 0$ in the strong coupling limit up to third order in t/U, starting from the Néel-state (i.e. the exact ground state for $t/U \to 0$ [9]). This yields the first terms of a (t/U)-expansion of the ground state energy, sublattice magnetization and momentum distribution.

DISCUSSION

In the absence of tractable and systematic theoretical techniques for the investigation of quantum mechanical many-body systems, it is useful to find particular limits in which these systems can be treated exactly. In this paper we discussed two such limits: infinite range hopping and high dimensionality. Within a short time the limit of infinite dimensions for correlated lattice fermions has turned out to be an especially fruitful approach. While correlations in the many-body system remain non-trivial, theoretical investigations become significantly simpler than in finite dimensions. This fact, in conjunction with explicit 1/d-corrections, gives rise to great hopes for the success of future theoretical investigations of correlated many-body systems in dimensions $1 < d < \infty$.

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