Variational investigation of low dimensional correlated electron systems via the limit of high dimensions

Rainer Strack, Dieter Vollhardt

Angaben zur Veröffentlichung / Publication details:

Strack, Rainer, and Dieter Vollhardt. 1991. "Variational investigation of low dimensional correlated electron systems via the limit of high dimensions." *Journal of Low Temperature Physics* 84 (5-6): 357–80. https://doi.org/10.1007/bf00683525.

Variational Investigation of Low Dimensional Correlated Electron Systems via the Limit of High Dimensions*

Rainer Strack and Dieter Vollhardt

Institut für Theoretische Physik C, Technische Hochschule Aachen, D-5100 Aachen, Germany

We show that the limit of large dimensions ($d=\infty$) can be used to obtain accurate variational results even for low dimensional ($d=1$, 2) fermionic systems, such as the Hubbard model or the periodic Anderson model. Using explicit correlated variational wave functions this is achieved by evaluating the expectation values for $d=\infty$ with the correct d-dimensional density of states and including 1/d-corrections. For example, an application of this approach to the periodic Anderson model in $d=1$ shows that the result for the ground state energy, the momentum distributions of c- and f-electrons, and the spin-spin and density-density correlations functions for the f-electrons are in excellent agreement with the variational Monte Carlo data of Shiba.

1. INTRODUCTION

Variational wave functions (VWFs) are well recognized as useful and versatile instruments for investigating interacting many-body systems.[1] They have recently received a particular attention in the study of heavy fermion systems and high-T_c superconductivity. These involve strongly correlated electrons with short-range repulsion, where conventional methods, e.g. perturbation theory, are often not applicable. The microscopic models chosen to investigate the abovementioned systems are usually of the Hubbard-type, i.e. an essential part of the interaction is described by an on-site repulsion of two electrons with different spin. In this case Gutzwiller-type VWFs[2,3] are the natural starting point for a variational treatment. In spite of their simple structure, analytic evaluations of expectation values in terms of these wave functions are generally not tractable, an exception being the simple Gutzwiller wave function in dimension $d=1$.[4] Even the scope of numerical evaluations is strongly limited by the number of variational

*Dedicated to L. Tewordt on the occasion of his 65th birthday.

parameters entering the wave function. In this situation the limit of *high* spatial dimensions ($d \to \infty$), which has recently been introduced by Metzner and Vollhardt[5] for the investigation of fermionic lattice models, has turned out to be a particularly useful approach: although Hubbard-type and their correlations remain nontrivial, actual calculations become much simpler.[6] Since then the limit $d = \infty$ has been applied to a number of problems involving the variational evaluation of ground state properties of the Hubbard model and the periodic Anderson model.[3,7-13] Corrections to the results in $d = \infty$ have also been obtained.[7] In particular, Gebhard[8,9] has developed a highly efficient formalism for the systematic calculation of $1/d$-corrections. In the case of the paramagnetic Gutzwiller wave function he showed that the numerical results for $d = 2, 3$ by Yokoyama and Shiba[14,15] and even the exact evaluations in $d = 1$,[4] are well described by the analytic results for $d = \infty$, when (low order) $1/d$-corrections are included (see also Ref. 7).

In the present paper the results described above will be extended in two directions: (i) we calculate the $1/d$-corrections to the ground state energy of the Hubbard model in $d = \infty$ for the projected spin density (i.e. antiferromagnetic Hartree-Fock) wave function; (ii) for the periodic Anderson model the appropriately generalized paramagnetic Gutzwiller wave function[16,17] is used to calculate the spin–spin and density–density correlation functions of the f-electron for $d = \infty$, as well as the ground state energy and momentum distributions in $d = \infty$ including $1/d$-corrections. The results are then applied to $d = 1$, using the correct density of states in $d = 1$. We find that the results from the large d limit, which can be obtained analytically, are in excellent agreement with variational Monte-Carlo results obtained for $d = 1$.[15,18,19] This shows that the large d limit is, in fact, a particularly useful limit for variational investigations in terms of Gutzwiller-type wave functions, since it yields very good quantitative results even in *low* dimensions, where analytic evaluations are not tractable.

2. VARIATIONAL APPROACH TO THE HUBBARD MODEL

2.1. Model and Wave Function

We first address the Hubbard model, $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_U$, for nearest neighbor hopping where

$$\hat{H}_{\text{kin}} = -t \sum_{\langle \mathbf{ij} \rangle, \sigma} \hat{c}^{+}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{a}^{+}_{\mathbf{k}\sigma} \hat{a}_{\mathbf{k}\sigma} \tag{2.1}$$

$$\hat{H}_U = U\hat{D} = U \sum_{\mathbf{i}} \hat{D}_{\mathbf{i}} = U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} \tag{2.2}$$

Here $\hat{c}^{+}_{\mathbf{i}\sigma}$ ($\hat{c}_{\mathbf{i}\sigma}$) creates (annihilates) a particle with spin σ on site $\mathbf{i}$, their Fourier transforms being given by $\hat{a}^{+}_{\mathbf{k}\sigma}$ ($\hat{a}_{\mathbf{k}\sigma}$). The corresponding number

operators are $\hat{n}_{i\sigma} = \hat{c}^{+}_{i\sigma}\hat{c}_{i\sigma}$ and $\hat{n}_{k\sigma} = \hat{a}^{+}_{k\sigma}\hat{a}_{k\sigma}$. The operator $\hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ counts the double occupancy at site i. In the limit of high dimensions d the parameter t must be scaled as[5]

$$t = \frac{t^*}{\sqrt{2d}} \tag{2.3}$$

to obtain a nontrivial model for $d \to \infty$. Therefore, the dispersion relation takes the form

$$\varepsilon_k = -\frac{2}{\sqrt{2d}} \sum_{i=1}^{d} \cos k_i \tag{2.4}$$

where we set $t^* = 1$.

To calculate expectation values of ground state properties of the Hubbard model Gutzwiller[2] introduced the variational wave function[3]

$$|\Psi_g\rangle = g^{\hat{D}}|\Psi_0\rangle = \prod_i [1-(1-g)\hat{D}_i]|\Psi_0\rangle \tag{2.5}$$

where $|\Psi_0\rangle$ is a one-particle (product) wave function; originally $|\Psi_0\rangle$ was taken to be the paramagnetic Fermi sea.[2] Here g is a variational parameter which is determined by the minimum of the energy expectation value. For increasing repulsion U the "Gutzwiller correlator" $g^{\hat{D}}$ reduces the amplitude of those spin configurations in $|\Psi_0\rangle$ with too many doubly occupied sites; thereby it introduces genuine correlations into $|\Psi_0\rangle$.

2.2. Diagrammatic Formulation

A diagrammatic formalism for the evaluation of expectation values in terms of $|\Psi_g\rangle$, taking into account the simplifying features of the on-site Hubbard interaction, was worked out by Metzner and Vollhardt.[4,5,7] In the limit $d \to \infty$ drastic simplifications occur, whereby an exact analytic evaluation of expectation values becomes possible. This formalism was cast into a particularly efficient form by Gebhard,[8,9] where in $d = \infty$ *all* diagrams reduce to zero, and $1/d$-corrections can be calculated rather simply. This can be achieved if one does not work with $|\Psi_g\rangle$ in the form given by (2.5), where the (square of the) Gutzwiller correlator has the form

$$g^{2\hat{D}} = \prod_i [1+(g^2-1)\hat{D}_i] \tag{2.6}$$

but, rather, by working relative to Hartree-Fock, using the expansion

$$g^{2\hat{K}} = \prod_i [1+x_i(\hat{D}_i - \hat{D}_i^{HF})] \tag{2.7}$$

with

$$\hat{K} = \hat{D} - \sum_i (\mu_{i\uparrow}\hat{n}_{i\uparrow} + \mu_{i\downarrow}\hat{n}_{i\downarrow} - \eta_i) \tag{2.8}$$

Here $\hat{D}_i^{HF} = \hat{n}_{i\uparrow}\langle\hat{n}_{i\downarrow}\rangle_0 + \hat{n}_{i\downarrow}\langle\hat{n}_{i\uparrow}\rangle_0 - \langle\hat{n}_{i\uparrow}\rangle_0\langle\hat{n}_{i\downarrow}\rangle_0$ is the Hartree-Fock decomposition of $\hat{D}_i$. Thereby, the variation wave function takes the form

$$|\Psi_g\rangle = g^{\hat{K}}|\Phi_0\rangle \tag{2.9}$$

with

$$|\Phi_0\rangle = g^{\hat{D}-\hat{K}}|\Psi_0\rangle \tag{2.10}$$

Of course, $|\Phi_0\rangle$ is also a one-particle wave function—just as $|\Psi_0\rangle$, since $g^{\hat{D}-\hat{K}}$ does not introduce any correlations between the particles, but only considers local "fugacities". The parameters x_i, $\mu_{i\uparrow}$, $\mu_{i\downarrow}$, and η_i are functions of g, $n_{i,0} = \langle\hat{n}_{i\uparrow}\rangle_0 + \langle\hat{n}_{i\downarrow}\rangle_0$, $m_{i,0} = \langle\hat{n}_{i\uparrow}\rangle_0 - \langle\hat{n}_{i\downarrow}\rangle_0$, and $\bar{d}_{i,0} = \langle\hat{n}_{i\uparrow}\rangle_0\langle\hat{n}_{i\downarrow}\rangle_0$ and are given by

$$\begin{aligned} x_i = & \frac{1}{2(1-g^2)\bar{d}_{i,0}(1-n_{i,0}+\bar{d}_{i,0})} \\ & \times\Big[-1+(1-g^2)(n_{i,0}-2\bar{d}_{i,0}) \\ & +\sqrt{1+(g^2-1)[n_{i,0}(2-n_{i,0})+g^2 m_{i,0}^2]}\Big] \end{aligned} \tag{2.11a}$$

$$g^{2\eta_i} = 1 + x_i\bar{d}_{i,0} \tag{2.11b}$$

$$g^{-2\mu_{i\sigma}} = 1 - \frac{x_i\langle\hat{n}_{i-\sigma}\rangle_0}{1+x_i\bar{d}_{i,0}} \tag{2.11c}$$

The expectation values with subscript zero are calculated in terms of $|\Phi_0\rangle$; note that $|\Psi_0\rangle \equiv |\Phi_0\rangle$ for $g = 1$.

In the original formalism,[4,5,7] where $|\Psi_g\rangle$ was used in the form (2.5), all diagrammatic elements were composed of the one-particle density matrix of the uncorrelated system ($g = 1$) $P_\sigma^0(\mathbf{i},\mathbf{j}) = \langle\Psi_0|\hat{c}_{i\sigma}^+\hat{c}_{j\sigma}|\Psi_0\rangle$, corresponding to *lines*, and the numbers g^2-1, corresponding to *vertices*. For $\mathbf{i} = \mathbf{j}$ one has $P_\sigma^0(\mathbf{i},\mathbf{i}) \neq 0$. However, in Gebhard's formulation[9] lines correspond to $\tilde{P}_\sigma^0(\mathbf{i},\mathbf{j}) = (1-\delta_{i,j})P_\sigma^0(\mathbf{i},\mathbf{j})$, with $P_\sigma^0(\mathbf{i},\mathbf{j}) = \langle\hat{c}_{i\sigma}^+\hat{c}_{j\sigma}\rangle_0$, and vertices correspond to the numbers x_i, i.e. are site-dependent in general. This has the great advantage that the diagonal elements of $\tilde{P}_\sigma^0$ vanish: $\tilde{P}_\sigma^0(\mathbf{i},\mathbf{i}) = 0$. Note that the *form* of the diagrams in both formulations is identical.

To obtain the one-particle density matrix $P_\sigma(\mathbf{i},\mathbf{j}) = \langle\hat{c}_{i\sigma}^+\hat{c}_{j\sigma}\rangle$ and the double occupancy $\bar{d}_i = \langle\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\rangle$ at site $\mathbf{i}$ in terms of $|\Psi_g\rangle$ as given by (2.9), it is useful to introduce a quantity $\tilde{S}_\sigma(\mathbf{i},\mathbf{j})$ whose diagrammatic representation in terms of $\tilde{P}_\sigma^0(\mathbf{i},\mathbf{j})$ and x_i corresponds to the usual self-energy diagrams in a ϕ^4-theory. This self-energy is given by

$$\begin{aligned} \tilde{S}_0(\mathbf{g},\mathbf{h}) = & -x_g\delta_{g,h}\{(n_{g-\sigma}-\langle\hat{n}_{g-\sigma}\rangle_0)\tilde{\mathscr{D}}\}_0^c \\ & + x_g x_h\{c_{g\sigma}^+ c_{h\sigma}(n_{g-\sigma}-\langle\hat{n}_{g-\sigma}\rangle_0)(n_{h-\sigma}-\langle\hat{n}_{h-\sigma}\rangle_0)\tilde{\mathscr{D}}\}_0^c \end{aligned} \tag{2.12}$$

with

$$\tilde{\mathscr{D}} = 1 + \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{\mathbf{g}_1 \ldots \mathbf{g}_m} x_{\mathbf{g}_1} \ldots x_{\mathbf{g}m} (D_{\mathbf{g}_1} - D_{\mathbf{g}_1}^{HF}) \ldots (D_{\mathbf{g}_m} - D_{\mathbf{g}_m}^{HF}) \quad (2.13)$$

where $\{\ldots\}_0^c$ denotes the sum over all possible pairs of contractions. Only those pairs that belong to connected graphs contribute.

In terms of the self energy the expectation values have the form[9]

$$P_\sigma(\mathbf{i}, \mathbf{j}) = \sqrt{q_{\mathbf{i}\sigma}} \sqrt{q_{\mathbf{j}\sigma}} \left[\tilde{P}_\sigma^0(\mathbf{i}, \mathbf{j}) + \sum_{\mathbf{g},\mathbf{h}} (\tilde{P}_\sigma^0(\mathbf{i}, \mathbf{g}) - \delta_{\mathbf{i},\mathbf{g}} \alpha_{\mathbf{i}\sigma}) \times \tilde{S}_\sigma(\mathbf{g}, \mathbf{h}) (\tilde{P}_\sigma^0(\mathbf{h}, \mathbf{j}) - \delta_{\mathbf{h},\mathbf{j}} \alpha_{\mathbf{j}\sigma}) \right] \quad (2.14a)$$

$$\langle \hat{n}_{\mathbf{i}\sigma} \rangle = \langle \hat{n}_{\mathbf{i}\sigma} \rangle_0 - \frac{1}{x_\mathbf{i}} \tilde{S}_{-\sigma}(\mathbf{i}, \mathbf{i}) - (1 - \langle \hat{n}_{\mathbf{i}\sigma} \rangle_0) \langle \hat{n}_{\mathbf{i}\sigma} \rangle_0 \tilde{S}_\sigma(\mathbf{i}, \mathbf{i}) - (1 - 2\langle \hat{n}_{\mathbf{i}\sigma} \rangle_0) \sum_{\mathbf{f}} \tilde{S}_\sigma(\mathbf{i}, \mathbf{f}) \tilde{P}_\sigma^0(\mathbf{f}, \mathbf{i}) \quad (2.14b)$$

$$\bar{d}_\mathbf{i} = [1 + x_\mathbf{i}(1 - n_{\mathbf{i},0} + \bar{d}_{\mathbf{i},0})] \times \left\{ \bar{d}_{\mathbf{i},0} - \frac{1}{x_\mathbf{i}} \sum_\sigma \left[\langle \hat{n}_{\mathbf{i}\sigma} \rangle_0 \tilde{S}_\sigma(\mathbf{i}, \mathbf{i}) + \tfrac{1}{2}(1 - x_\mathbf{i} \bar{d}_{\mathbf{i},0}) \sum_{\mathbf{f}} \tilde{S}_\sigma(\mathbf{i}, \mathbf{f}) \tilde{P}_\sigma^0(\mathbf{f}, \mathbf{i}) \right] \right\} \quad (2.14c)$$

The quantities $\sqrt{q_{\mathbf{i}\sigma}}$ and $\alpha_{\mathbf{i}\sigma}$ are determined by the following equations:

$$\sqrt{q_{\mathbf{i}\sigma}} = g^{2\eta_\mathbf{i}} g^{-\mu_{\mathbf{i}\sigma}} [1 + \langle \hat{n}_{\mathbf{i}-\sigma} \rangle_0 (g^{1-2\mu_{\mathbf{i}-\sigma}} - 1)] \quad (2.15a)$$

$$\alpha_{\mathbf{i}\sigma} = \frac{g^{1-2\mu_{\mathbf{i}-\sigma}} - 1}{x_\mathbf{i}[1 + \langle \hat{n}_{\mathbf{i}-\sigma} \rangle_0 (g^{1-2\mu_{\mathbf{i}-\sigma}} - 1)]} \quad (2.15b)$$

These relations are valid in any dimension. The first nonvanishing diagram of the self energy (it is of 2nd order) is shown in Fig. 1.

On a d-dimensional hypercubic lattice with $d \to \infty$ one has[5,7] $P_\sigma^0(\mathbf{i}, \mathbf{j}) \simeq \mathcal{O}([\sqrt{1/d}]^\nu)$, where $\nu = |\mathbf{i} - \mathbf{j}| = \sum_{l=1}^d |i_l - j_l|$ is the so-called "New York" metric.[12] It counts the number of nearest neighbor steps from $\mathbf{i}$ to $\mathbf{j}$. Due

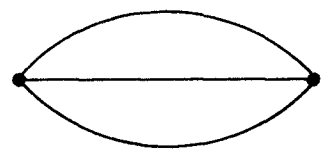

Fig. 1. Self energy diagram (second order) leading to $1/d$-correction.

to this fact all self energy diagrams, i.e. the self energy itself, *vanish* in the limit $d = \infty$

$$\lim_{d \to \infty} \tilde{S}_\sigma(\mathbf{g}, \mathbf{h}) = 0 \tag{2.16}$$

Hence, in $d = \infty$ one obtains the simple, exact result[9]

$$P_\sigma(\mathbf{i}, \mathbf{j}) = \sqrt{q_{\mathbf{i}\sigma}}\sqrt{q_{\mathbf{j}\sigma}}\,\tilde{P}^0_\sigma(\mathbf{i}, \mathbf{j}) \qquad \mathbf{i} \neq \mathbf{j} \tag{2.17}$$

and the expectation value of the Hubbard Hamiltonian is given by

$$\langle \hat{H} \rangle = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \sum_\sigma \sqrt{q_{\mathbf{i}\sigma}}\sqrt{q_{\mathbf{j}\sigma}}\, P^0_\sigma(\mathbf{i}, \mathbf{j}) + U \sum_{\mathbf{i}} \bar{d}_{\mathbf{i}} \tag{2.18}$$

Equation (2.18) was first obtained by Kotliar and Ruckenstein[20] within a slave-boson approach. The factors $\sqrt{q_{\mathbf{i}\sigma}}$ describe a *local* renormalization of hopping processes.

2.3. $1/d$-Corrections

Next, we want to calculate $1/d$-corrections to the $d = \infty$ result; to this end we have to consider $1/d$-corrections to the variational parameters. In the simplest case the Hamiltonian depends only on one variational parameter x

$$\langle \hat{H} \rangle = a_0(x) + a_1(x)\left(\frac{1}{d}\right) + \mathcal{O}\left(\frac{1}{d^2}\right) \tag{2.19}$$

x is determined by minimizing $\langle \hat{H} \rangle$. The $1/d$-expansion of x is given by $x = x^{(0)} + x^{(1)}(1/d) + \mathcal{O}((1/d)^2)$. It follows immediately that

$$\langle \hat{H} \rangle = a_0(x^{(0)}) + a_1(x^{(0)})\left(\frac{1}{d}\right) + \mathcal{O}\left(\frac{1}{d^2}\right) \tag{2.20}$$

i.e. the expectation value of the energy to order $(1/d)$ is determined by $x^{(0)}$, the optimal value of x in $d = \infty$. This statement also holds in the case of more than one variational parameter.

3. THE GUTZWILLER-PROJECTED SPIN-DENSITY WAVE FUNCTION

The formalism described above will now be applied in the case of a Gutzwiller projected wave function with antiferromagnetic long range order (AFLRO). To this end $|\Psi_0\rangle$ in (2.5) is chosen to be the antiferromagnetic

Hartree-Fock wave function ($n_\uparrow = n_\downarrow = \frac{1}{2}$)

$$|\Psi_{0,AF}\rangle = \prod_{\sigma} \prod_{\varepsilon_{\mathbf{k}} \leq 0} [u_{\mathbf{k}} \hat{a}^+_{\mathbf{k}\sigma} + \sigma v_{\mathbf{k}} \hat{a}^+_{\mathbf{k}+\mathbf{Q}\sigma}]|0\rangle \tag{3.1a}$$

Here $\mathbf{Q} = (\pi, \pi, \ldots, \pi)$ is half a reciprocal lattice vector, and

$$u_{\mathbf{k}} = \frac{1}{\sqrt{2}} [1 + \sqrt{1 - \theta^2_{\mathbf{k}}}]^{1/2} \tag{3.1b}$$

$$v_{\mathbf{k}} = -\mathrm{sgn}(\varepsilon_{\mathbf{k}}) \frac{1}{\sqrt{2}} [1 - \sqrt{1 - \theta^2_{\mathbf{k}}}]^{1/2} \tag{3.1c}$$

are determined by

$$\theta_{\mathbf{k}} = \frac{\Delta}{\sqrt{\varepsilon^2_{\mathbf{k}} + \Delta^2}} \tag{3.1d}$$

with $\Delta = \frac{1}{2} Um$ and m as the sublattice magnetization.

It is interesting to note that for AB-type lattices, where $\varepsilon_{\mathbf{k}} = -\varepsilon_{\mathbf{k}+\mathbf{Q}}$, $|\Psi_{0,AF}\rangle$ in (2.1) can be written in the form

$$|\Psi_{0,AF}\rangle = e^{\hat{T}} |\text{Néel}\rangle \tag{3.2a}$$

where $|\text{Néel}\rangle$ is the Néel-state and $\hat{T}$ has the form of a kinetic energy operator

$$\hat{T} = \sum_{\mathbf{k}\sigma} \tilde{\varepsilon}_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma} \tag{3.2b}$$

with

$$\tilde{\varepsilon}_{\mathbf{k}} = \tfrac{1}{2} \ln \left[\frac{\varepsilon_{\mathbf{k}}}{\Delta} + \sqrt{1 + \left(\frac{\varepsilon_{\mathbf{k}}}{\Delta} \right)^2} \right] \tag{3.2c}$$

and $\tilde{\varepsilon}_{\mathbf{k}} = -\tilde{\varepsilon}_{\mathbf{k}+\mathbf{Q}}$. The operator in (3.2a) acting on $|\text{Néel}\rangle$ has the form of a correlation operator. It introduces hopping processes into the localized Néel-state,[21] i.e. reduces the perfect Néel-order and leads precisely to the Hartree-Fock wave function (3.1a) having AFLRO. Hence this correlator favors hopping, while the Gutzwiller correlator $\exp(\ln g \hat{D})$ does just the opposite. The Gutzwiller correlated wave function based on (3.1a) can then be written as

$$|\Psi_{g,AF}\rangle = g^{\hat{D}} e^{\hat{T}} |\text{Néel}\rangle \tag{3.3}$$

Since it is more convenient to work with (2.9) than (2.5), we need $|\Phi_{0,AF}\rangle$, rather than $|\Psi_{0,AF}\rangle$, as the starting wave function with AFLRO. In fact, $|\Phi_{0,AF}\rangle$ can be expressed as in (3.1a) with $\theta_{\mathbf{k}}$ replaced by a new variational function $\tilde{\theta}_{\mathbf{k}} (= \tilde{\theta}_{\mathbf{k}+\mathbf{Q}})$;[9] of course, $\theta_{\mathbf{k}} = \tilde{\theta}_{\mathbf{k}}$ for $g = 1$.

3.1. $d=\infty$

In $d=\infty$ the self energy $\tilde{S}_\sigma$, (2.16), vanishes and therefore one finds[9] for the expectation value of the energy, (2.18),

$$\langle \hat{H} \rangle^\infty = 2q(m_0, \bar{d}^\infty) \sum_{\varepsilon_{\mathbf{k}} \leq 0} \varepsilon_{\mathbf{k}} \sqrt{1-\tilde{\theta}_{\mathbf{k}}^2} + UL\bar{d}^\infty \tag{3.4}$$

with

$$q(m_0, \bar{d}^\infty) = \frac{\bar{d}^\infty}{d_0} \{2\sqrt{(\bar{d}^\infty)^2 - \bar{d}^\infty + d_0} + (1-2\bar{d}^\infty)\} \tag{3.5}$$

Note, that in the case under investigation $\bar{d}_i \equiv \bar{d}$ is site independent; here $\bar{d}^\infty$ is the density of doubly occupied sites of the correlated state in $d=\infty$, and d_0 is that for the noninteracting system. The vertex x_i is given by $x_i = x = (\bar{d}^\infty - \bar{d}_0)/\bar{d}_0^2$. Here we take $\bar{d}^\infty$ instead of g as the new variational parameter. Minimization of the energy with respect to the function $\tilde{\theta}_{\mathbf{k}}$ (infinitely many variational parameters!) yields

$$\tilde{\theta}_{\mathbf{k}} = \tilde{\theta}_{\mathbf{k}}^\infty = \frac{\Delta}{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta^2}} \tag{3.6}$$

with a new $\mathbf{k}$-independent variational parameter Δ. Hence, the minimization problem has been reduced to a *two*-parameter problem. It is interesting to see that $\tilde{\theta}_{\mathbf{k}}$ maintains its Hartree-Fock form even after the Gutzwiller-correlator has been switched on ($g<1$)! This is only true in $d=\infty$.

3.2. $1/d$-Corrections to the Self Energy

To account for the broken translational invariance we introduce the following Fourier representation of the self energy

$$\tilde{S}_\sigma(\mathbf{i}, \mathbf{j}) = \frac{2}{L} \sum_{\mathbf{k} \in MB} e^{-i\mathbf{k}(\mathbf{i}-\mathbf{j})} \tilde{S}_\sigma^{XY}(\mathbf{k}) \tag{3.7}$$

where $\mathbf{i} \in X$-sublattice and $\mathbf{j} \in Y$-sublattice and $\mathbf{k}$ is an element of the first magnetic Brillouin zone (MB), i.e. that Brillouin zone which corresponds to the reduced translational invariance of the sublattice. The inverse transformation is given by

$$\tilde{S}_\sigma^{XY}(\mathbf{k}) = \frac{2}{L} \sum_{\mathbf{i} \in X, \mathbf{j} \in Y} e^{i\mathbf{k}(\mathbf{i}-\mathbf{j})} \tilde{S}_\sigma(\mathbf{i}, \mathbf{j}) \tag{3.8}$$

The quantities $\tilde{S}_\sigma^{XY}(\mathbf{k})$ can be arranged in a matrix[7]

$$\tilde{\mathbf{S}}_\sigma(\mathbf{k}) = \begin{bmatrix} \tilde{S}_\sigma^{AA}(\mathbf{k}) & \tilde{S}_\sigma^{AB}(\mathbf{k}) \\ \tilde{S}_\sigma^{BA}(\mathbf{k}) & \tilde{S}_\sigma^{BB}(\mathbf{k}) \end{bmatrix} \tag{3.9}$$

$P^0_\sigma(\mathbf{i},\mathbf{j})$ can be transformed similarly, where $\mathbf{k}\in MB$,

$$\mathbf{P}^0_\sigma(\mathbf{k})=\chi_{\mathbf{k}}\begin{bmatrix}\frac{1}{2}(1+\sigma\tilde{\theta}_{\mathbf{k}}) & \frac{1}{2}\sqrt{1-\tilde{\theta}^2_{\mathbf{k}}}\\ \frac{1}{2}\sqrt{1-\tilde{\theta}^2_{\mathbf{k}}} & \frac{1}{2}(1-\sigma\tilde{\theta}_{\mathbf{k}})\end{bmatrix} \tag{3.10}$$

with $\chi_{\mathbf{k}}=1$ for $\varepsilon_{\mathbf{k}}\le 0$, otherwise $\chi_{\mathbf{k}}=0$. Note, that for a quantity $C_{\mathbf{ij}}=\sum_{\mathbf{g}} A_{\mathbf{ig}}B_{\mathbf{gj}}$ the convolution theorem reads

$$\mathbf{C}(\mathbf{k})=\mathbf{A}(\mathbf{k})\mathbf{B}(\mathbf{k}) \tag{3.11}$$

where $\mathbf{A}(\mathbf{k})\mathbf{B}(\mathbf{k})$ is the matrix product of $\mathbf{A}(\mathbf{k})$ and $\mathbf{B}(\mathbf{k})$.

The only graph contributing to the off-diagonal part of the self energy to order $(1/d)$ is shown in Fig. 1 where $\mathbf{i}$ is a next neighbor of $\mathbf{j}$ ($\mathbf{i}=\mathbf{j}+\boldsymbol{\tau}$)

$$\tilde{S}_\sigma(\mathbf{i},\mathbf{j})=-x^2P^0_\sigma(\mathbf{i},\mathbf{j})[P^0_{-\sigma}(\mathbf{i},\mathbf{j})]^2\delta_{\mathbf{i}-\mathbf{j},\boldsymbol{\tau}} \tag{3.12}$$

with $P^0_\sigma(\mathbf{i},\mathbf{i}+\boldsymbol{\tau})=-\bar{\varepsilon}/(2\sqrt{2d})$ where $\bar{\varepsilon}$ is the average kinetic energy of the non-interacting system

$$\bar{\varepsilon}=\frac{2}{L}\sum_{\varepsilon_{\mathbf{k}}\le 0}\varepsilon_{\mathbf{k}}\sqrt{1-\tilde{\theta}^2_{\mathbf{k}}} \tag{3.13}$$

The diagonal part of the self energy can be calculated by use of particle conservation $\langle\hat{n}_{\mathbf{i}\sigma}\rangle+\langle\hat{n}_{\mathbf{i}-\sigma}\rangle=\langle\hat{n}_{\mathbf{i}\sigma}\rangle_0+\langle\hat{n}_{\mathbf{i}-\sigma}\rangle_0$ and the equation $\tilde{S}_{-\sigma}(\mathbf{i},\mathbf{i})=-x_{\mathbf{i}}\sum_{\mathbf{g},\mathbf{h}}\tilde{P}^0_\sigma(\mathbf{i},\mathbf{g})\tilde{S}_\sigma(\mathbf{g},\mathbf{h})\tilde{P}^0_\sigma(\mathbf{h},\mathbf{i})$.

Finally, we obtain for the self energy

$$\tilde{S}^{AB}_\sigma(\mathbf{k})=-\frac{x^2\bar{\varepsilon}^2\varepsilon_{\mathbf{k}}}{16d} \tag{3.14a}$$

$$\tilde{S}^{AA}_\sigma(\mathbf{k})=\left(\frac{x\bar{\varepsilon}}{4\sqrt{d}}\right)^2\frac{b^\sigma_+a^\sigma_- - p_\sigma b^\sigma_-}{a^\sigma_+a^\sigma_- - p^2_\sigma} \tag{3.14b}$$

with

$$\left.\begin{aligned} b^\sigma_s&=\langle\hat{n}^s_\sigma\rangle_0\bar{\varepsilon}-\frac{1}{2L}\sum_{\varepsilon_{\mathbf{k}}\le 0}\varepsilon_{\mathbf{k}}(1+s\sigma\tilde{\theta}_{\mathbf{k}})\\ a^\sigma_s&=\langle\hat{n}^s_\sigma\rangle^2_0-\frac{1}{4L}\sum_{\varepsilon_{\mathbf{k}}\le 0}\varepsilon_{\mathbf{k}}(1+s\sigma\tilde{\theta}_{\mathbf{k}})^2\end{aligned}\right\}\ s=+,- \tag{3.15a}$$

$$p_\sigma=-\frac{1}{x}-\frac{1}{4L}\sum_{\varepsilon_{\mathbf{k}}\le 0}\varepsilon_{\mathbf{k}}(1-\sigma\tilde{\theta}^2_{\mathbf{k}}) \tag{3.15b}$$

Here $\langle\hat{n}^+_\sigma\rangle_0$, $\langle\hat{n}^-_\sigma\rangle_0$ are the particle densities on the A-and B-sublattice in the uncorrelated state, respectively. We find $\tilde{S}^{AB}_\sigma(\mathbf{k})=\tilde{S}^{BA}_\sigma(\mathbf{k})$ and $\tilde{S}^{AA}_\sigma(\mathbf{k})=\tilde{S}^{BB}_{-\sigma}(\mathbf{k})$.

3.3. Ground State Energy with $1/d$-Corrections

Using the self energy (3.14) we obtain for the ground state energy of the Hubbard model up to, and including, the order $(1/d)$

$$\begin{aligned}\langle \hat{H} \rangle = 2q(m_0, \bar{d}^\infty)\Bigg(& \sum_{\varepsilon_{\mathbf{k}} \leqslant 0} \varepsilon_{\mathbf{k}} \sqrt{1-\tilde{\theta}_{\mathbf{k}}^{\infty 2}} \\ & + 2 \sum_{k \in MB} \varepsilon_{\mathbf{k}} \{ [\mathbf{P}_\sigma^0(\mathbf{k}) - (\alpha_\sigma^A + \langle \hat{n}_\sigma^A \rangle_0)\mathbf{1}] \tilde{\mathbf{S}}_\sigma(\mathbf{k}) \\ & \times [\mathbf{P}_\sigma^0(\mathbf{k}) - (\alpha_\sigma^B + \langle \hat{n}_\sigma^B \rangle_0)\mathbf{1}] \}_{12} \Bigg) \\ & + LU\bar{d}^\infty \Bigg(1 - \frac{\bar{d}_0}{\bar{d}^\infty - \bar{d}_0} \Bigg[\tfrac{1}{2}(1+m_0)\tilde{S}_\uparrow^{AA}(\mathbf{k}) + \tfrac{1}{2}(1-m_0)\tilde{S}_\uparrow^{BB}(\mathbf{k}) \\ & - \tfrac{1}{2}(1 - x\bar{d}_0) \frac{S\bar{\varepsilon}}{d} \Bigg] \Bigg) \end{aligned} \tag{3.16}$$

with

$$\tilde{\theta}_{\mathbf{k}}^\infty = \frac{\Delta}{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta^2}} \tag{3.17}$$

Here Δ and $\bar{d}^\infty$ are given by the $d = \infty$ result and $S = (x\bar{\varepsilon}/4)^2$. All quantities are calculated with these two variational parameters. Note that $\{\mathbf{A}\}_{12} = A_{12}$.

3.4. Application to Finite Dimensions

The ground state energy of the Hubbard model in $d = \infty$ in terms of $|\Psi_{g,AF}\rangle$ was evaluated already by Metzner.[7] Comparison with the uncorrelated Hartree–Fock result for $d = \infty$ showed that both results are numerically very close, i.e. the additional correlation effects due to the Gutzwiller correlator lower then energy only by a small amount in this case. The variational Monte-Carlo (VMC) results of Yokoyama and Shiba[15] indicate that this is true even in dimensions $d = 2$ and 3; only in $d = 1$ do they find a somewhat larger discrepancy between the results for the correlated and the uncorrelated wave function.

We will now use the results for the ground state energy derived above, which are the exact evaluations for $d = \infty$, to obtain an *approximation* for lower dimensions. At this point it should be mentioned that $1/d$-corrections to the results for $d = \infty$ do not only come from the diagrammatic contributions calculated so far, but also from the expansion of the density of states (DOS) that enters in the $\mathbf{k}$-(or energy) integrals.[22,23] Besides that there exist *nonanalytic* corrections to the DOS of order $e^{-\alpha d}$ due to van Hove singularities. To avoid difficulties arising from such corrections we use the *exact* d-dimensional DOS, in addition to the explicit $1/d$-corrections due

to diagrams, to obtain results for a finite dimensional system. If we include corrections of order $1/d$ from diagrams, the error introduced thereby is of order $(1/d)^2$. This scheme will now be applied to obtain results in $d=1$, which—in principle—will be the hardest for us to describe, since the validity of the approximation is least certain in this case. The applicability of these results to the case $d=1$ is therefore a priori uncertain.

In Fig. 2 we compare various results for the ground state energy E/L ($L=$ number of lattice sites) of the Hubbard model in $d=1$: (i) the exact result by Lieb and Wu,[24] (ii) the VMC result for $|\Psi_{g,AF}\rangle$ of Ref. 15, (iii) the result for $|\Psi_{g,AF}\rangle$, obtained analytically for $d=\infty$, but evaluated with the correct DOS for $d=1$, (iv) the results for this wave function including $1/d$-corrections due to diagrams, and, (v) the conventional Hartree-Fock result ($g=1$ in (3.3)). Obviously the $1/d$-correction, evaluated for $d=1$, moves the curve away from the $d=\infty$ result into the right direction and gives full agreement with the numerical data for $U\lesssim 3$. (The deviations at larger U can be understood by noting that $\tilde{S}_\sigma(\mathbf{k})$, which determines the $1/d$-correction, is given by an expansion in $(n/2)^2 x$, which is very small only for small densities or interactions U.) It must also be mentioned that the authors of Ref. 15 *assumed* $\theta_\mathbf{k}$ in (3.1) to be given by the Hartree-Fock form (3.1d) even for the correlated wave function with $g\neq 1$, to reduce the numerics to a two-parameter problem. However, for the wave function

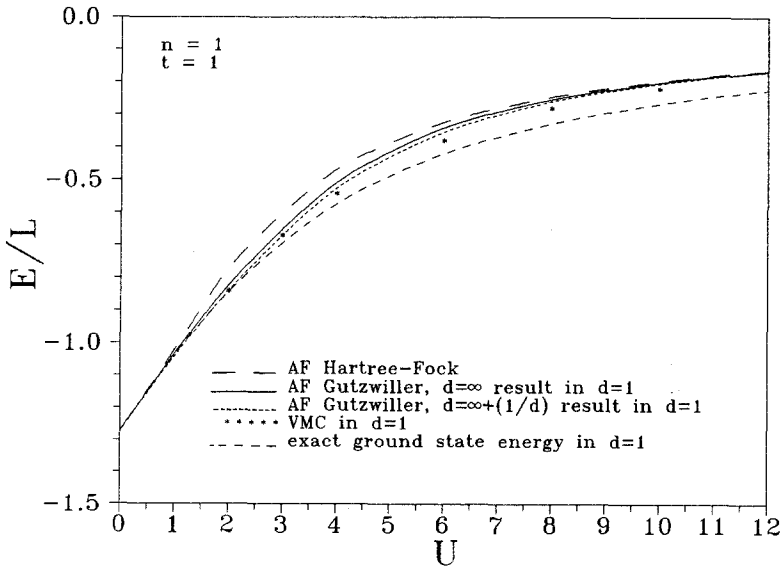

Fig. 2. Ground state energy of the Hubbard model versus interaction U in $d=1$. Variational results of increasing refinement are compared with numerical evaluations[15] (VMC) and the exact[24] result.

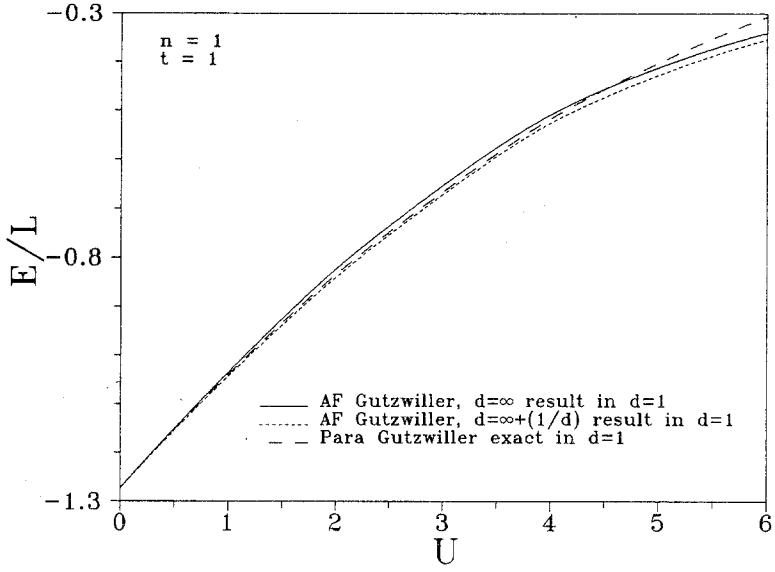

Fig. 3. Ground state energy of the Hubbard model versus U for different variational wave functions in $d = 1$. The qualitative importance of the $1/d$-correction for $U \lesssim 4.5$ is apparent (see text).

$|\Psi_{g,AF}\rangle$ expressed by (2.5) this assumption is never warranted—not even in $d = \infty$;[5,7] it is only correct for $\tilde{\theta}_k$, i.e. when $|\Psi_{g,AF}\rangle$ is written in the form (2.9), in $d = \infty$.[9] Nevertheless, the error introduced by this assumption does not seem to be significant in the present case. We see that the $1/d$-correction leads to quantitative improvements for all U. As shown in Fig. 3 this correction is also of *qualitative* importance: without $1/d$-correction the energy for the paramagnetic Gutzwiller wave function becomes *lower* than the antiferromagnetic VMF for $U \lesssim 4.5$, suggesting a phase transition. However, the $1/d$-correction lowers the energy of the antiferromagnetically correlated state below that of the paramagnetic one for *all* $U > 0$, as one should expect. Numerical values of the energy can, of course, easily be calculated also for dimensions $d = 2, 3$. In these dimensions the agreement will be even better. Hence the variational approach to low dimensions via the limit $d \to \infty$ is seen to yield very good quantitative results in dimensions as low as $d = 1$.

4. VARIATIONAL APPROACH TO THE PERIODIC ANDERSON MODEL

The periodic Anderson model (PAM) is used to describe physical properties of mixed-valence compounds and heavy fermion systems.[25] In

its simplest version it consists of a band of delocalized conduction electrons which hybridize with strongly localized f-electrons. The interaction between the f-electrons is modelled by a Hubbard interaction. In this case the Hamilton operator (PAM) is given by

$$\begin{aligned}\hat{H}_{\mathrm{PAM}} &= \sum_{\mathbf{k}\sigma} \varepsilon_c(\mathbf{k})\hat{n}^c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \varepsilon_f(\mathbf{k})\hat{n}^f_{\mathbf{k}\sigma} \\ &\quad - \sum_{\mathbf{k}\sigma} V_{\mathbf{k}}(\hat{f}^+_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} + \hat{c}^+_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma}) + U\sum_{\mathbf{i}} \hat{n}^f_{\mathbf{i}\uparrow}\hat{n}^f_{\mathbf{i}\downarrow} \\ &= \hat{H}^c_{kin} + \hat{H}^f_{kin} + \hat{H}_{hyb} + \hat{H}^f_U \end{aligned} \tag{4.1}$$

Here $\hat{c}^+_{\mathbf{i}\sigma}$ and $\hat{f}^+_{\mathbf{i}\sigma}$ creates a c- and f-electron, respectively, with spin σ on site $\mathbf{i}$, and $\hat{n}^f_{\mathbf{i}\sigma} = \hat{f}^+_{\mathbf{i}\sigma}\hat{f}_{\mathbf{i}\sigma}$ etc. Their counterparts in momentum space are now written as $\hat{c}^+_{\mathbf{k}\sigma}$ and $\hat{f}^+_{\mathbf{k}\sigma}$ for simplicity, where $\mathbf{k}$ is the momentum, with $\hat{n}^c_{\mathbf{k}\sigma} = \hat{c}^+_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}$, $\hat{n}^f_{\mathbf{k}\sigma} = \hat{f}^+_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma}$.The kinetic energy of the c- and f-electrons is parameterized by $\varepsilon_c(\mathbf{k})$ and $\varepsilon_f(\mathbf{k})$, respectively, and $V_{\mathbf{k}}$ is the hybridzation matrix element. For $U = 0$ the ground state is given by ($n \leqslant 2$)

$$|\Psi_{0,\mathrm{PAM}}\rangle = \prod_{\mathbf{k}\sigma} [1 + a^0_{\mathbf{k}\sigma}\hat{f}^+_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}]|cFS\rangle \tag{4.2}$$

where

$$a^0_{\mathbf{k}\sigma} = \frac{2V_k}{\varepsilon_f(\mathbf{k}) - \varepsilon_c(\mathbf{k}) + \sqrt{(\varepsilon_c(\mathbf{k}) - \varepsilon_f(\mathbf{k}))^2 + 4V^2_{\mathbf{k}}}} \tag{4.3}$$

and

$$|cFS\rangle = \prod_{\varepsilon_c(\mathbf{k}) \leqslant \varepsilon_F, \sigma} \hat{c}^+_{\mathbf{k}\sigma}|\mathrm{vacuum}\rangle \tag{4.4}$$

is the Fermi sea of the conduction electrons if an f-level is not occupied. In the following we consider the dispersion (2.4) for $\varepsilon_c(\mathbf{k})$, as well as $\varepsilon_f(\mathbf{k}) = E_f = \mathrm{const}$, $V_{\mathbf{k}} = V = \mathrm{const}$.

In view of the Hubbard interaction between the f-electrons it is natural to introduce correlations into $|\Psi_{0,\mathrm{PAM}}\rangle$ via a Gutzwiller correlator for the f-electrons[16,17] in analogy with (2.5), (2.9). The Gutzwiller wave function for the PAM is then given by

$$|\Psi_g\rangle = g^{\hat{D}^f}|\Psi_{0,\mathrm{PAM}}\rangle \tag{4.5}$$

$$= g^{\hat{K}^f}|\Phi_{0,\mathrm{PAM}}\rangle \tag{4.6}$$

with[8,9]

$$|\Phi_{0,\mathrm{PAM}}\rangle = g^{\sum_i(\mu_{i\uparrow}\hat{n}^f_{i\uparrow} + \mu_{i\downarrow}\hat{n}^f_{i\downarrow} - \eta_i)}|\Psi_{0,\mathrm{PAM}}\rangle \tag{4.7}$$

One obtains for $|\Phi_0\rangle$

$$|\Phi_{0,\mathrm{PAM}}\rangle = \prod_{\mathbf{k}\sigma} [1 + \tilde{a}_{\mathbf{k}\sigma}\hat{f}^+_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}]|cFS\rangle \tag{4.8}$$

with

$$\tilde{a}_{\mathbf{k}\sigma} = g^{\mu_\sigma}a^0_{\mathbf{k}\sigma} \tag{4.9}$$

Here $\tilde{a}_{\mathbf{k}\sigma}$ is taken as a new variational function to account for the fact that the hybridization will be changed by the interaction. Hence $\tilde{a}_{\mathbf{k}\sigma}$ and g are to be determined variationally. Expectation values in the uncorrelated state are calculated with $|\Phi_{0,\mathrm{PAM}}\rangle$.

Since the Gutzwiller correlator contains only f-electron operators the expectation values must be transformed in such a way that only f-electrons appear. Again we introduce the self energy $\tilde{S}_\sigma(\mathbf{i},\mathbf{j})$, which now only refers to f-electron operators. Here we consider the strongly correlated limit $U=\infty$, i.e. $\bar{d}_\mathbf{i}^f=0$, $g=0$.

Due to translational invariance and spin symmetry of the wave function, one obtains for $x_\mathbf{i}$, $\sqrt{q_\mathbf{i}}$, and $\alpha_\mathbf{i}$ (Refs. 8, 26):

$$x_\mathbf{i}=x=-\frac{4}{(2-n_0^f)^2} \tag{4.10}$$

$$\sqrt{q_\mathbf{i}}=\sqrt{q}=\sqrt{\frac{1-n_0^f}{1-n_0^f/2}} \tag{4.11}$$

$$\alpha_\mathbf{i}=\alpha=1-\frac{n_0^f}{2} \tag{4.12}$$

where n_0^f is the f-electron density in the uncorrelated state. We transform all calculations of expectation values into momentum space because of translational invariance. Introducing the Fourier transform of the self energy

$$\tilde{S}_\sigma(\mathbf{k})=\frac{1}{L}\sum_{\mathbf{i},\mathbf{j}} e^{i\mathbf{k}(\mathbf{i}-\mathbf{j})}\tilde{S}_\sigma(\mathbf{i},\mathbf{j}) \tag{4.13}$$

One obtains the following $n(\mathbf{k})$ distributions:

$$\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle=q\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle_0+\frac{n_0^f}{2}(1-q)+q\left[\left(\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle_0-\frac{n_0^f}{2}-\alpha\right)^2\tilde{S}_\sigma(\mathbf{k})\right.$$
$$\left.-\frac{1}{L}\sum_\mathbf{k}\left(\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle_0-\frac{n_0^f}{2}-\alpha\right)^2\tilde{S}_\sigma(\mathbf{k})\right] \tag{4.14}$$

$$\langle\hat{n}_{\mathbf{k}\sigma}^c\rangle=\langle\hat{n}_{\mathbf{k}\sigma}^c\rangle_0+\langle\hat{n}_{\mathbf{k}\sigma}^x\rangle_0^2\tilde{S}_\sigma(\mathbf{k}) \tag{4.15}$$

$$\langle\hat{n}_{\mathbf{k}\sigma}^x\rangle=\langle\hat{f}_{\mathbf{k}\sigma}^+\hat{c}_{\mathbf{k}\sigma}\rangle=\sqrt{q}\left[\langle\hat{n}_{\mathbf{k}\sigma}^x\rangle_0+\left(\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle_0-\frac{n_0^f}{2}-\alpha\right)\langle\hat{n}_{\mathbf{k}\sigma}^x\rangle_0\tilde{S}_\sigma(\mathbf{k})\right] \tag{4.16}$$

Hence, the expectation value of the Hamiltonian is given by

$$\langle\hat{H}_{\mathrm{PAM}}\rangle=\sum_{\mathbf{k}\sigma}\left[\varepsilon_c(\mathbf{k})\langle\hat{n}_{\mathbf{k}\sigma}^c\rangle_0+E_f\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle_0-2V\sqrt{q}\,\langle\hat{n}_{\mathbf{k}\sigma}^x\rangle_0\right]$$
$$+\sum_{\mathbf{k}\sigma}\tilde{S}_\sigma(\mathbf{k})\left[\varepsilon_c(\mathbf{k})\langle\hat{n}_{\mathbf{k}\sigma}^x\rangle_0^2-2V\sqrt{q}\left(\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle_0-\frac{n_0^f}{2}-\alpha\right)\langle\hat{n}_{\mathbf{k}\sigma}^x\rangle_0\right]$$
$$+\lambda\left\{Ln_0^f-\sum_{\mathbf{k}\sigma}\langle\hat{n}_{\mathbf{k}\sigma}^f\rangle_0\right\} \tag{4.17}$$

Here a Lagrange multiplier λ was introduced to be able to vary $\tilde{a}_{\mathbf{k}\sigma}$ and n_0^f independently. These equations are valid in every dimension d.

4.1. $d=\infty$

For $d=\infty$ the results have already been obtained by Gebhard[8,26] (for a preliminary account see Ref. 13). Since the self energy vanishes in $d=\infty$ (see (2.15a)) the result for $\langle \hat{H}_{\mathrm{PAM}} \rangle$ in (4.17) implies that the Gutzwiller correlator in (4.5), (4.6) only leads to the following *renormalization* of the model parameters for the noninteracting system:

$$V \to \sqrt{q}\, V \tag{4.18a}$$

$$E_f \to E_f - \lambda^{\infty} \tag{4.18b}$$

(for the general $\mathbf{k}$- and σ-dependent case see Refs. 8, 13). Hence the variational problem for determining $\tilde{a}_{\mathbf{k}\sigma}$ is formally identical to that for $U=0$. For the correlated case one therefore finds

$$\tilde{a}_{\mathbf{k}\sigma} = a_{\mathbf{k}\sigma}^{\infty} = \frac{2V\sqrt{q}}{(E_f - \varepsilon_c(\mathbf{k}) - \lambda^{\infty}) + \sqrt{(E_f - \varepsilon_c(\mathbf{k}) - \lambda^{\infty})^2 + 4V^2 q}} \tag{4.19}$$

The above results had already been found earlier by several groups[16,27-29] within a Gutzwiller *approximation* (semi-classical counting of spin configurations) and a slave boson approach.[20] These approximate evaluations are hence seen to become exact in the limit $d=\infty$.

4.2. $1/d$-Corrections to the Self Energy

In Fig. 1 the only graph contributing to the off-diagonal part of the self energy to order $(1/d)$ is shown, where $\mathbf{i}$ is a nearest neighbor of $\mathbf{j}$ ($\mathbf{i}=\mathbf{j}+\boldsymbol{\tau}$). It is given by

$$\tilde{S}_{\sigma}(\mathbf{i},\mathbf{j}) = -x^2 [P_{\sigma}^{f,0}(\mathbf{i},\mathbf{j})]^3 \delta_{\mathbf{i}-\mathbf{j},\boldsymbol{\tau}} \tag{4.20}$$

with $P_{\sigma}^{f,0}(\mathbf{i},\mathbf{i}+\boldsymbol{\tau}) = -\bar{\varepsilon}_1/(2\sqrt{2d})$ and

$$\bar{\varepsilon}_1 = \frac{2}{L}\sum_{\mathbf{k}} \varepsilon_c(\mathbf{k}) \langle \hat{n}_{\mathbf{k}\sigma}^f \rangle_0 \tag{4.21}$$

By use of particle conservation of the c- and f-electrons $\langle \hat{n}_{\mathbf{i}\sigma}^f \rangle + \langle \hat{n}_{\mathbf{i}\sigma}^c \rangle = \langle \hat{n}_{\mathbf{i}\sigma}^f \rangle_0 + \langle \hat{n}_{\mathbf{i}\sigma}^c \rangle_0$, the diagonal part of the self energy is now determined to order $(1/d)$. Hence, we obtain for $\tilde{S}_{\sigma}(\mathbf{k})$

$$\tilde{S}_{\sigma}(\mathbf{k}) = \frac{x^2 \bar{\varepsilon}_1^3}{16d}\left\{ \frac{-(1-n_0^f)\bar{\varepsilon}_1/2 + \bar{\varepsilon}_2/2}{(1/L)\sum_{\mathbf{k}} \langle \hat{n}_{\mathbf{k}\sigma}^x \rangle_0^2 - [1/x + (1-n_0^f/2)n_0^f/2]} - \varepsilon_c(\mathbf{k}) \right\} \tag{4.22}$$

with

$$\bar{\varepsilon}_2 = \frac{2}{L}\sum_{\mathbf{k}} \varepsilon_c(\mathbf{k}) \langle \hat{n}_{\mathbf{k}\sigma}^x \rangle_0^2 \tag{4.23}$$

4.3. Ground State Energy with $1/d$-Corrections

To be consistent in $1/d$ we must take the $1/d$-expansions of $\tilde{a}_{\mathbf{k}\sigma}$, n_0^f, and λ into account

$$\tilde{a}_{\mathbf{k}\sigma} = a_{\mathbf{k}\sigma}^{\infty} + \frac{1}{d} b_{\mathbf{k}\sigma} + \mathcal{O}\left(\frac{1}{d^2}\right) \tag{4.24a}$$

$$n_0^f = n_0^{f\infty} + \frac{1}{d} n_0^{f(1/d)} + \mathcal{O}\left(\frac{1}{d^2}\right) \tag{4.24b}$$

$$\lambda = \lambda^{\infty} + \frac{1}{d} \lambda^{(1/d)} + \mathcal{O}\left(\frac{1}{d^2}\right) \tag{4.24c}$$

Again the expectation value of the energy including the $1/d$-correction is completely determined by the parameters in $d = \infty$:

$$\begin{aligned}\langle \hat{H}_{\mathrm{PAM}} \rangle = & \sum_{\varepsilon_c(\mathbf{k}) \geq \varepsilon_{F\sigma}} \frac{\varepsilon_c(\mathbf{k}) a_{\mathbf{k}\sigma}^{\infty 2} + (E_f - \lambda^{\infty}) a_{\mathbf{k}\sigma}^{\infty 2} - 2V\sqrt{q}\,|_{n_0^{f\infty}} a_{\mathbf{k}\sigma}^{\infty}}{1 + a_{\mathbf{k}\sigma}^{\infty 2}} \\ & + \sum_{\varepsilon_c(\mathbf{k}) \leq \varepsilon_{F\sigma}} \tilde{S}_{\sigma}(\mathbf{k})|_{a_{\mathbf{k}\sigma}^{\infty}, n_0^{f\infty}, \lambda^{\infty}} \frac{\varepsilon_c(\mathbf{k}) a_{\mathbf{k}\sigma}^{\infty 2} + 2V\sqrt{q}\,|_{n_0^{f\infty}} a_{\mathbf{k}\sigma}^{\infty}}{(1 + a_{\mathbf{k}\sigma}^{\infty 2})^2} \\ & + \lambda^{\infty} L n_0^{f\infty}. \end{aligned} \tag{4.25}$$

4.4. Momentum Distributions with $1/d$-Corrections

For the c- and f-electrons we obtain

$$\langle \hat{n}_{\mathbf{k}\sigma}^c \rangle = \langle \hat{n}_{\mathbf{k}\sigma}^c \rangle_0 + \frac{\partial \langle \hat{n}_{\mathbf{k}\sigma}^c \rangle_0}{\partial \tilde{a}_{\mathbf{k}\sigma}} \frac{b_{\mathbf{k}\sigma}}{d} + \tilde{S}_{\sigma}(\mathbf{k}) \langle \hat{n}_{\mathbf{k}\sigma}^x \rangle_0^2 + \mathcal{O}\left(\frac{1}{d^2}\right) \tag{4.26}$$

$$\begin{aligned}\langle \hat{n}_{\mathbf{k}\sigma}^f \rangle = & q \langle \hat{n}_{\mathbf{k}\sigma}^f \rangle_0 + \frac{\partial q(n_0^f)}{\partial n_0^f} \langle \hat{n}_{\mathbf{k}\sigma}^f \rangle_0 \frac{n_0^{f(1/d)}}{d} + q \frac{\partial \langle \hat{n}_{\mathbf{k}\sigma}^f \rangle_0}{\partial \tilde{a}_{\mathbf{k}\sigma}} \frac{b_{\mathbf{k}\sigma}}{d} \\ & + \frac{n_0^{f\infty}}{2}(1-q) + \frac{n_0^{f(1/d)}}{2d}(1-q) - \frac{n_0^{f\infty}}{2} \frac{\partial q(n_0^f)}{\partial n_0^f} \frac{n_0^{f(1/d)}}{d} \\ & + q \left[\left(\langle \hat{n}_{\mathbf{k}\sigma}^f \rangle_0 - \frac{n_0^{f\infty}}{2} - \alpha \right)^2 \tilde{S}_{\sigma}(\mathbf{k}) \right. \\ & \left. - \frac{1}{L} \sum_{\mathbf{k}} \left(\langle \hat{n}_{\mathbf{k}\sigma}^f \rangle_0 - \frac{n_0^{f\infty}}{2} - \alpha \right)^2 \tilde{S}_{\sigma}(\mathbf{k}) \right] + \mathcal{O}\left(\frac{1}{d^2}\right) \end{aligned} \tag{4.27}$$

All quantities are calculated with the parameters $a_{\mathbf{k}\sigma}^{\infty}$, $n_0^{f\infty}$, and λ^{∞}.

4.5. Correlation Functions for the f-Electrons in $d=\infty$

To investigate the magnetic and charge correlations among the f-electrons for infinite U, we now calculate the spin-spin and density-density correlation functions in terms of $|\Psi_{g,\mathrm{PAM}}\rangle$. In real space the correlation functions (CF) are defined by[30]

$$C^{XX}(\mathbf{j})=\frac{1}{L}\sum_{\mathbf{i}}\{\langle\hat{X}_{\mathbf{i}}\hat{X}_{\mathbf{i}+\mathbf{j}}\rangle-\langle\hat{X}_{\mathbf{i}}\rangle\langle\hat{X}_{\mathbf{i}+\mathbf{j}}\rangle\} \tag{4.28}$$

with

$$\hat{X}_{\mathbf{i}}=\begin{cases}\hat{S}^{f,z}_{\mathbf{i}}=\hat{n}^{f}_{\mathbf{i}\uparrow}-\hat{n}^{f}_{\mathbf{i}\downarrow} & \text{(spin)}\\ \hat{N}^{f}_{\mathbf{i}}=\hat{n}^{f}_{\mathbf{i}\uparrow}+\hat{n}^{f}_{\mathbf{i}\downarrow} & \text{(density)}\end{cases} \tag{4.29}$$

For the Hubbard model in $d=\infty$ these CFs were calculated by van Dongen *et al.*[12] One finds that they are entirely determined by RPA-type bubbles in this case, i.e. remain nontrivial in the limit $d=\infty$. In Gebhard's formulation the spin-spin and density-density CFs are given by (35a, b) of Ref. 9. If we interpret the densities $\hat{n}_{\mathbf{i}\sigma}$ etc. entering in these equations as f-electrons densities, the expressions can be directly used for our purpose. In $d=\infty$ and for $g=0$ we therefore have

$$c^{S^zS^z}(\mathbf{j})=\frac{1}{L}\frac{4}{(2-n_0^f)^2}\sum_{\mathbf{i}\sigma}\{\tilde{Y}^{(1)}_{\sigma}(\mathbf{i},\mathbf{i}+\mathbf{j})-\tilde{Y}^{(4)}_{\sigma}(\mathbf{i},\mathbf{i}+\mathbf{j})\} \tag{4.30}$$

$$C^{NN}(\mathbf{j})=\frac{4}{L}\frac{(1-n_0^f)^2}{(2-n_0^f)^2}\sum_{\mathbf{i}\sigma}\{\tilde{Y}^{(1)}_{\sigma}(\mathbf{i},\mathbf{i}+\mathbf{j})+\tilde{Y}^{(4)}_{\sigma}(\mathbf{i},\mathbf{i}+\mathbf{j})\} \tag{4.31}$$

where $\tilde{Y}^{(1)}_{\sigma}$ and $\tilde{Y}^{(4)}_{\sigma}$ are given by the consistency equations

$$\begin{aligned}\tilde{Y}^{(1)}_{\sigma}(\mathbf{g},\mathbf{h})&=-[\tilde{P}^{f,0}_{\sigma}(\mathbf{g},\mathbf{h})]^2\\&\quad+\sum_{\mathbf{lm}}x_{\mathbf{l}}x_{\mathbf{m}}[\tilde{P}^{f,0}_{\sigma}(\mathbf{g},\mathbf{l})]^2\tilde{Y}^{(1)}_{-\sigma}(\mathbf{l},\mathbf{m})[\tilde{P}^{f,0}_{\sigma}(\mathbf{m},\mathbf{h})]^2\end{aligned} \tag{4.32}$$

$$\begin{aligned}\tilde{Y}^{(4)}_{\sigma}(\mathbf{g},\mathbf{h})&=\sum_{\mathbf{l}}x_{\mathbf{l}}[\tilde{P}^{f,0}_{\sigma}(\mathbf{g},\mathbf{l})]^2[\tilde{P}^{f,0}_{-\sigma}(\mathbf{l},\mathbf{h})]^2\\&\quad+\sum_{\mathbf{lm}}x_{\mathbf{l}}x_{\mathbf{m}}[\tilde{P}^{f,0}_{\sigma}(\mathbf{g},\mathbf{l})]^2\tilde{Y}^{(4)}_{-\sigma}(\mathbf{l},\mathbf{m})[\tilde{P}^{f,0}_{-\sigma}(\mathbf{m},\mathbf{h})]^2\end{aligned} \tag{4.33}$$

which follow from summing the bubble diagrams (the only ones that remain in $d=\infty$). These expressions are now Fourier transformed according to $Z(\mathbf{q})=\sum_j e^{i\mathbf{q}\cdot\mathbf{j}}Z(\mathbf{i},\mathbf{i}+\mathbf{j})$, where $Z=C^{XX}$, $\tilde{Y}^{(1)}_{\sigma}$, $\tilde{Y}^{(4)}_{\sigma}$. From this it follows that

$$\tilde{Y}^{(4)}_{\sigma}(\mathbf{q})=\frac{x[\Delta\Pi_0(\mathbf{q})]^2}{1-x^2[\Delta\Pi_0(\mathbf{q})]^2}=-x\Delta\Pi_0(\mathbf{q})\,\tilde{Y}^{(1)}_{\sigma}(\mathbf{q}) \tag{4.34}$$

where

$$\Delta\Pi_0(\mathbf{q}) = \sum_{\mathbf{j}} e^{i\mathbf{q}\mathbf{j}}[\tilde{P}^0_\sigma(\mathbf{i}, \mathbf{i}+\mathbf{j})]^2 \tag{4.35}$$

Since the CFs for $\mathbf{j}=0$ are known, their Fourier transform finally follows as

$$C^{S^zS^z}(\mathbf{q}) = n_0^f - \frac{8}{(2-n_0^f)^2}\frac{\Delta\Pi_0(\mathbf{q})}{1-x\Delta\Pi_0(\mathbf{q})} + \frac{8}{(2-n_0^f)^2}\frac{1}{L}\sum_{\mathbf{q}}\frac{\Delta\Pi_0(\mathbf{q})}{1-x\Delta\Pi_0(\mathbf{q})} \tag{4.36a}$$

$$C^{NN}(\mathbf{q}) = n_0^f - n_0^{f^2} - \frac{8(1-n_0^f)^2}{(2-n_0^f)^2}\frac{\Delta\Pi_0(\mathbf{q})}{1+x\Delta\Pi_0(\mathbf{q})} + \frac{8(1-n_0^f)^2}{(2-n_0^f)^2}\frac{1}{L}\sum_{\mathbf{q}}\frac{\Delta\Pi_0(\mathbf{q})}{1+x\Delta\Pi_0(\mathbf{q})} \tag{4.36b}$$

where $\Delta\Pi_0(\mathbf{q})$ is determined by

$$\Delta\Pi_0(\mathbf{q}) = \frac{1}{L}\sum_{\mathbf{k}}\langle\hat{n}^f_{\mathbf{k}\sigma}\rangle_0\langle\hat{n}^f_{\mathbf{q}-\mathbf{k}\sigma}\rangle_0 - \frac{n_0^{f^2}}{4} \tag{4.37}$$

All quantities are calculated with the $d=\infty$ parameters $a^\infty_{\mathbf{k}\sigma}$, $n_0^{f\infty}$, and λ^∞.

4.6. Application to Finite Dimensions

To obtain an approximation for finite dimensions (see Sect. 3.4) the quantities calculated for the PAM in terms of $|\Psi_{g,\mathrm{PAM}}\rangle$ in the previous section (ground state energy, momentum distributions, correlation functions) are now evaluated for a given dimension d by using the exact d-dimensional DOS. We find that the actual numerical values obtained thereby do not depend on d very strongly. Of particular interest are the results for $d=1$, since this is the hardest dimension for us to reach and also because there exist numerical results (VMC), with which we can compare our results. We consider an equal number of up and down spins.

In Fig. 4 we show our results for the ground state energy of the PAM at $U=\infty$ as a function of n, the total density of c- and f-electrons. The results for $d=\infty$ and those including the $1/d$-correction are numerically very close and deviate only for densities $n \gtrsim 1.7$. The deviation at higher densities can be explained in the same way as in Sect. 3.4. These results are compared with VMC-results obtained for $|\Psi_{g,\mathrm{PAM}}\rangle$ at three different values of n: $n=1.5$ (Refs. 18, 31), $n=1.75$ (Ref. 18) and $n=2.0$ (Ref. 19). The

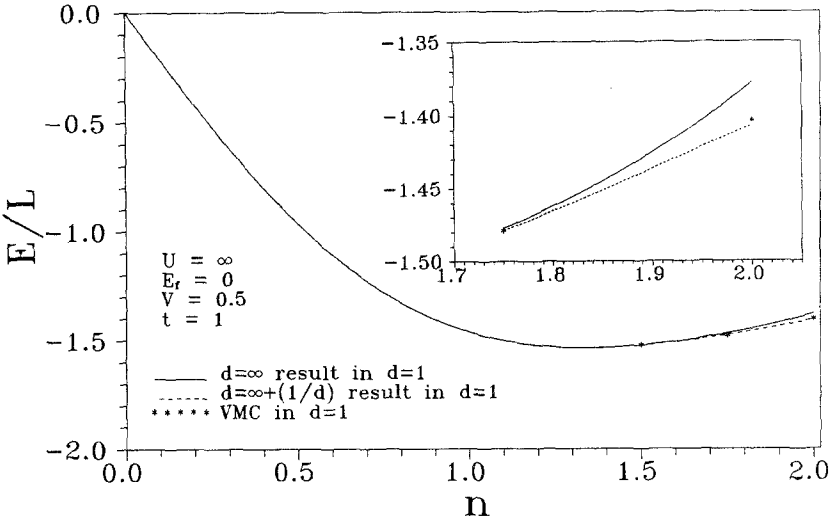

Fig. 4. Ground state energy of the periodic Anderson model versus total density n for the paramagnetic Gutzwiller wave function in $d = 1$ as compared with numerical evaluations[18,19,31] (VMC). In the insert the importance of the $1/d$-correction is made clear.

agreement is excellent. In particular, as shown in the insert, the $1/d$-correction brings the theoretical curve right on top of the numerical points.

In Fig. 5(a, b) our results for the momentum distributions in $d = 1$ of the c- and f-electrons at $U = \infty$ are shown for two different total densities n. At $n = 1.75$ there is still a Fermi surface at $k/\pi \cong 0.88$, suggesting metallic behavior. This must be considered an artefact, caused by the choice of the wave function, which is a projection onto the Fermi sea of the conduction electrons. Such a result is a typical property of paramagnetic Gutzwiller wave functions.[3,4] Only for $n = 2$, where the lower band is completely filled, is the Fermi surface absent. The theoretical curve are compared with the VMC results for $d = 1$ by Shiba.[18] For $n = 1.75$ the agreement is seen to be excellent; the $1/d$-correction has only a small effect. By contrast, for $n = 2$ the $1/d$-correction is signifiant. It moves the curves into the right direction, yielding excellent agreement again with the numerical points for $d = 1$, except for $k/\pi \gtrsim 0.7$ in the case of $n_{\mathbf{k}}^{c}$.

In Fig. 6(a-c) we show our results for the momentum dependence of the spin-spin and density-density correlation functions of the f-electrons in $d = 1$ at $U = \infty$ for different parameter values of the density n and the f-level energy E_f. Again the agreement with the VMC results by Shiba[18] is very good; the agreement is best for somewhat lower filling ($n < 2$) and not too low E_f. Even details like the discontinuity in C^{SS}, due to Umklapp

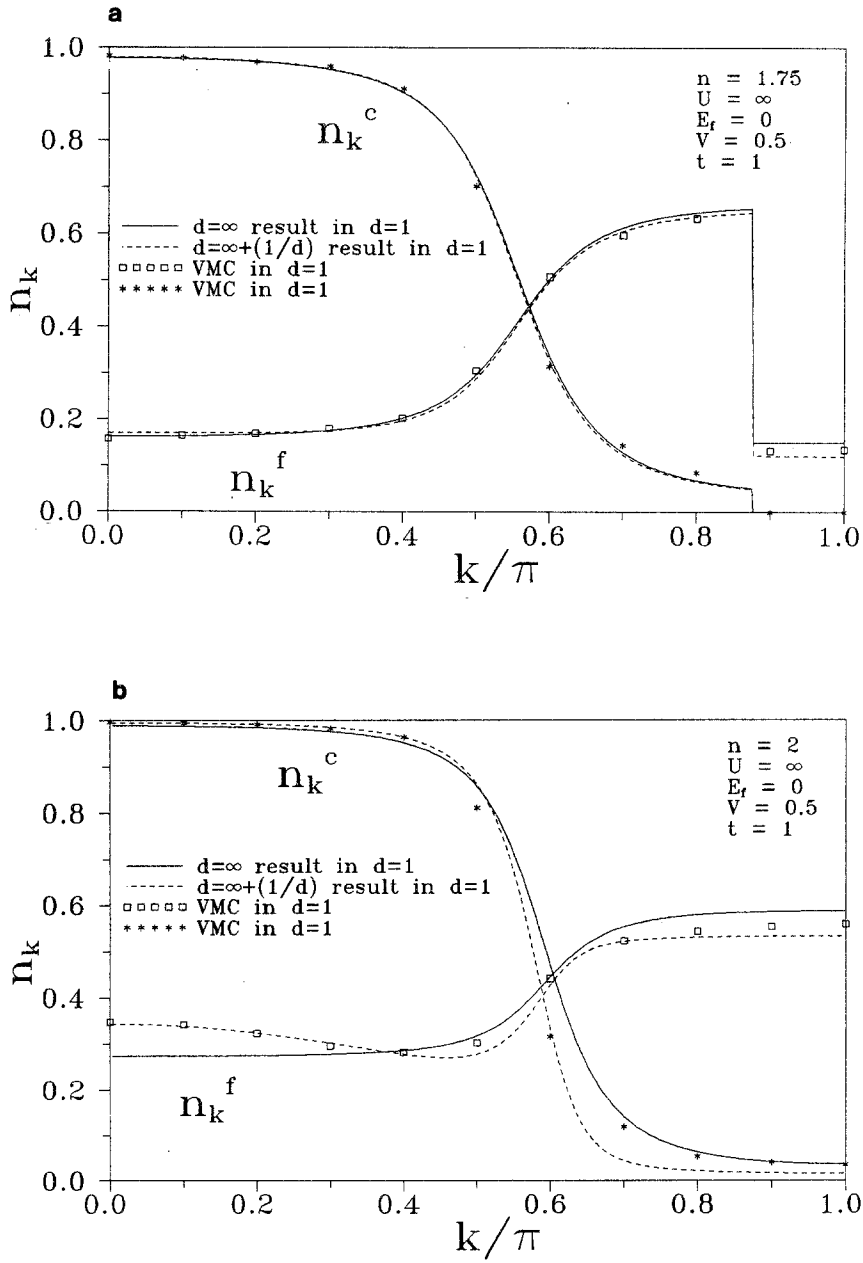

Fig. 5. Variational results for the momentum distributions n_k^c and n_k^f of the conduction and f-electrons, respectively, for the periodic Anderson model in $d = 1$. The numerical data by Shiba[18] are shown for comparison; (a) total density $n = 1.75$, (b) $n = 2.0$.

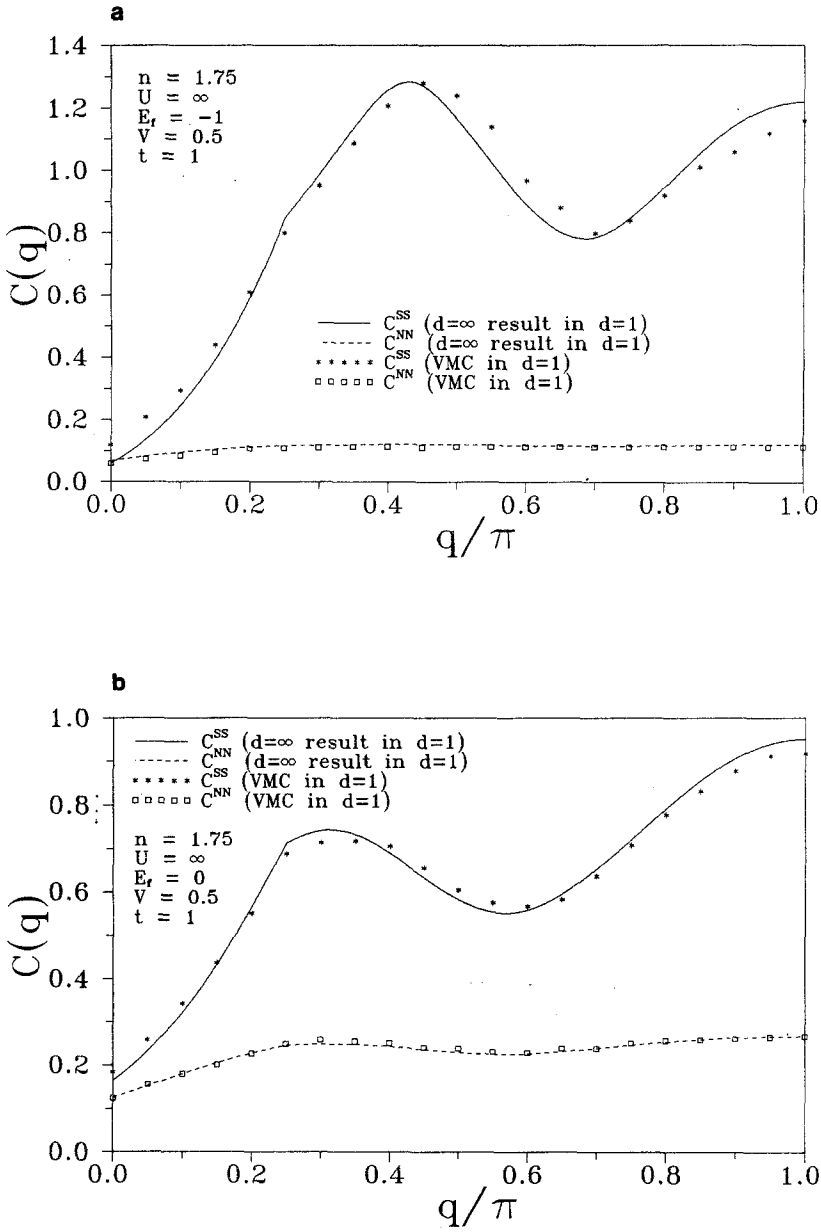

Fig. 6. Variational results for the momentum dependent spin-spin (C^{SS}) density-density (C^{NN}) correlation functions of the f-electrons in the $d = 1$ periodic Anderson model for various parameter values of n and E_f. The numerical data of Shiba[18] are shown for comparison. (a) $n = 1.75$, $E_f = -1$; (b) $n = 1.75$, $E_f = 0$; (c) $n = 2$, $E_f = 0$.

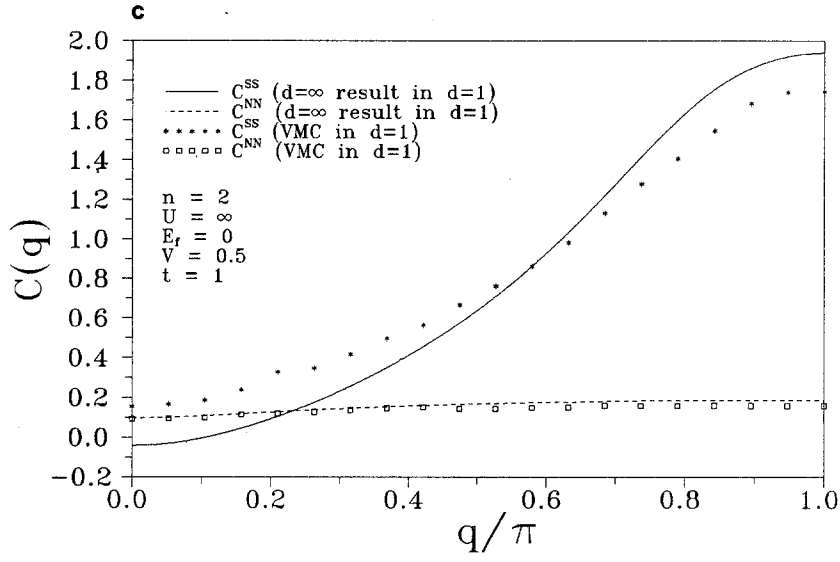

Fig. 6. Continued.

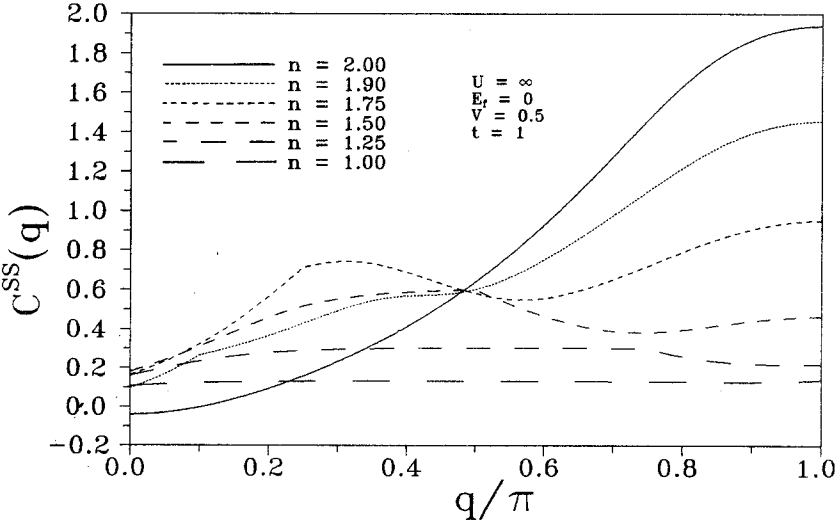

Fig. 7. Variational results for the f-electron spin-spin correlation function $C^{SS}(q)$ in the $d = 1$ periodic Anderson model for various values of the total density n.

processes at $q = 2(\pi - k_F)$, are clearly borne out. There is only little structure in C^{NN} due to the strong repulsion, while the spin degrees of freedom of the f-electrons do show considerable (antiferromagnetic) structure. InFig. 7 a family of curves for the spin–spin correlation function at various densities n is shown, indicating the onset of structure with increasing n.

5. DISCUSSION

In this paper we have investigated the Hubbard model and the periodic Anderson model using explicit correlated variational wave functions. Exact analytic evaluations of several quantities (ground state energy, momentum distribution, spin–spin and density–density correlation functions) have been performed in $d = \infty$ dimensions. This is the only dimension where such evaluations are tractable at all, made possible by the significant diagrammatic simplifications in this limit. In addition, $1/d$-corrections are calculated for some of these quantities. The results thus obtained where applied to *finite* dimensions d by making use of the exact d-dimensional density of states. Comparison with variational Monte-Carlo results for dimensions as low as $d = 1$ showed an excellent agreement. The $1/d$-corrections were found to be significant only at high particle densities; these corrections systematically improved the results. Our results clearly indicate that the limit of large dimensions d is a particularly helpful one in the case of variational investigations of finite-dimensional fermionic systems with Hubbard interaction. In this case correlations are known to remain nontrivial,[23,32] while at the same time analytic evaluations become feasible. As shown in our paper such evaluations may even be used to obtain *quantitatively* correct results for *low* dimensional systems. (This says nothing about the quality of the wave function in absolute terms.) The reason for this appears to lie in the nature of the variational wave functions under investigation: they are usually rather simple, being characterized by only a small number of variational parameters, with the symmetry of the wave function more or less determined by construction.

Therefore a reliable, practical strategy for any investigation in terms of Gutzwiller-correlated wave functions is to evaluate the quantities of interest in $d = \infty$ (this is always possible[5,9]) and then use the exact density of states in d dimensions to obtain a good approximation for the expectation values in this particular dimension.

ACKNOWLEDGMENTS

We are very grateful to Professor H. Shiba for providing us with unpublished data of his variational Monte Carlo studies of the periodic

Anderson model. We also wish to acknowledge helpful discussions with Dr. F. Gebhard and Dr. W. Metzner. One of us (R.S.) gratefully acknowledges a scholarship by the Studienstiftung des Deutschen Volkes. This work was supported in part by the Sonderforschungsbereich 341 of the Deutsche Forschungsgemeinschaft.

REFERENCES

1. For a brief review, see D. Vollhardt, in *Interacting Electrons in Reduced Dimensions*, eds. D. Baeriswyl and D. Campbell (Plenum Press, New York, 1989), p. 107.
2. M. C. Gutzwiller, *Phys. Rev. Lett.* **10**, 159 (1963); *Phys. Rev. A* **137**, 1726 (1965).
3. For a brief review, see D. Vollhardt, P. G. J. van Dongen, F. Gebhard, and W. Metzner, *Mod. Phys. Lett. B* **4**, 499 (1990).
4. W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **59**, 121 (1987); *Phys. Rev. B* **37**, 7382 (1988).
5. W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).
6. For recent reviews, see E. Müller-Hartmann, *Int. J. Mod. Phys. B* **3**, 2169 (1989); D. Vollhardt, *Physica B 169*, 277 (1991).
7. W. Metzner, *Z. Phys. B* **77**, 253 (1989).
8. F. Gebhard, Doctoral Thesis, RWTH Aachen, 1990 (unpublished).
9. F. Gebhard, *Phys. Rev. B* **41**, 9452 (1990).
10. P. Fazekas, B. Menge, and E. Müller-Hartmann, *Z. Phys. B* **78**, 69 (1990).
11. W. Metzner, *Z. Phys. B* **82**, 183 (1991).
12. P. van Dongen, F. Gebhard, and D. Vollhardt, *Z. Phys. B* **76**, 199 (1989).
13. F. Gebhard and D. Vollhardt, in *Interacting Electrons In Reduced Dimensions*, eds. D. Baeriswyl and D. Campbell (Plenum Press, New York, 1989), p. 123.
14. H. Yokoyama and H. Shiba, *J. Phys. Soc. Jpn*, **56**, 1490 (1987); **56**, 3570 (1987).
15. H. Yokoyama and H. Shiba, *J. Phys. Soc. Jpn.* **56**, 3582 (1987).
16. T. M. Rice and K. Ueda, *Phys. Rev. Lett.* **55**, 995 (1985); **55**, 2093 (*E*) (1985); *Phys. Rev.* **34**, 6420 (1986).
17. B. H. Brandow, *Phys. Rev. B* **33**, 215 (1986).
18. H. Shiba, *J. Phys. Soc. Jpn.* **55**, 2765 (1986).
19. 19. H. Shiba, private communication.
20. G. Kotliar and A. Ruckenstein, *Phys. Rev. Lett.* **57**, 1362 (1986).
21. This is similar to the approach by D. Baeriswyl [in *Nonlinearity in Condesnsed Matter*, eds. R. Bishop *et al.*, Springer Series in Solid State Sciences, Vol. 69 (Springer, Berlin 1987), p. 103] who thereby constructed a VWF for the $d = 1$ Hubbard model to lowest order in t/U.
22. U. Wolff, *Nucl. Phys. B* **225** , [FS9] 391 (1983).
23. E. Müller-Hartmann, *Z. Phys. B* **74**, 507 (1989).
24. E. H. Lieb and F. Y. Wu, *Phys. Rev. Lett.* **20**, 1445 (1968).
25. See for example, P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, *Comments Cond. Matt. Phys.* **12**, 99 (1986).
26. F. Gebhard, *Phys. Rev. B* **44**, 992 (1991).
27. C. M. Varma, W. Weber, and L. J. Randall, *Phys. Rev. B* **33**, 1015 (1985).
28. P. Fazekas and B. H. Brandow, *Phys. Scripta* **36**, 809 (1987).
29. V. Z. Vulović and E. Abrahams, *Phys. Rev. B* **36**, 2614 (1987).
30. F. Gebhard and D. Vollhardt, *Phys. Rev. Lett.* **59**, 1472 (1987); *Phys. Rev.* **37**, 7382 (1988).
31. T. Yanagisawa, *Phys. Rev. B* **37**, 2050 (1988).
32. P. van Dongen and D. Vollhardt, *Phys. Rev. Lett.* **65**, 1663 (1990).