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NEW VARIATIONAL APPROACH TO THE PERIODIC ANDERSON MODEL WITH ANTIFERROMAGNETIC ORDER

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We propose a new variational wave function for the periodic Anderson model in the case of antiferromagnetically ordered f-electrons. Expectation values in terms of this wave function can be calculated analytically in arbitrary dimensions d. The wave function automatically produces the exact limiting behavior of the ground state energy for weak hybridization and strong f-electron interaction in the symmetric case, which the Gutzwiller wave function fails to do. Several additional improvements are discussed. Thereby one obtains a wave function that leads to extremely good ground state energies for the periodic Anderson model for arbitrary U in all dimensions d.

1. Introduction

The physics of heavy-electron systems comprises many of the fundamental correlation-induced coherence phenomena known in condensed matter physics, such as magnetic order, superconductivity, Kondo effect, etc.[1] A comprehensive understanding of the origin of this fascinating wealth of physical properties not only requires a detailed theoretical understanding of each one of these phenomena, but also of their mutual influence. It is therefore not surprising that, in spite of intensive investigations over the last decade, many aspects are not yet adequately understood.

The simplest microscopic model describing essential features of heavy electron systems is the periodic Anderson model (PAM)

$$\hat{H}_{\mathrm{PAM}} = \sum_{\mathbf{k}\sigma} \varepsilon^c_{\mathbf{k}} \hat{n}^c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \varepsilon^f_{\mathbf{k}} \hat{n}^f_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} \hat{n}^f_{\mathbf{i}\uparrow} \hat{n}^f_{\mathbf{i}\downarrow} - \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} (\hat{f}^+_{\mathbf{k}\sigma}\, \hat{c}_{\mathbf{k}\sigma} + \hat{c}^+_{\mathbf{k}\sigma}\, \hat{f}_{\mathbf{k}\sigma}) \,. \quad (1)$$

It consists of strongly correlated, almost localized f-electrons ($\hat{f}$-operators) which are hybridized via the matrix $V_{\mathbf{k}}$ with a band of noninteracting conduction electrons ($\hat{c}$-operators) with energy dispersion $\varepsilon^c_{\mathbf{k}}$. In (1) the index $\mathbf{k}$ refers to momentum ($\hat{n}^c_{\mathbf{k}\sigma} = \hat{c}^+_{\mathbf{k}\sigma}\, \hat{c}_{\mathbf{k}\sigma}$) and $\mathbf{i}$ to lattice sites ($\hat{n}^f_{\mathbf{i}\sigma} = \hat{f}^+_{\mathbf{i}\sigma} \hat{f}_{\mathbf{i}\sigma}$). The interaction between the f-electrons is modelled by a Hubbard interaction U. For generality we have included in (1) a dispersion $\varepsilon^f_{\mathbf{k}}$ to allow for a (small) kinetic energy of the f-electrons. In the literature the f-electrons are usually considered to be localized ($U \to \infty$), such that $\varepsilon^f_{\mathbf{k}} \equiv E_f = \mathrm{const}$, and $V_{\mathbf{k}} \equiv V$ is chosen as constant, too.

In our paper we will address the U, V dependence of the ground state energy E_{PAM} of (1) for total electron density $n = 2$, using perturbational and variational methods. In particular, we will first point out a peculiar deficiency of the Gutzwiller wave function for the PAM,[2,3] namely that the corresponding ground state energy is systematically too high. We will then present a new type of correlated variational wave functions in terms of which expectation values can be evaluated *exactly* in any dimension $d = 1, 2, \ldots, \infty$, and which at the same time yields the exact asymptotic behavior at small V and large U for all d in the symmetric case.

2. Gutzwiller Wave Function for the PAM

In the non-interacting case ($U = 0$) the ground state wave function for (1) has the form

$$|\Psi_{\mathrm{PAM}}(U=0)\rangle \equiv |\Psi_{\mathrm{PAM},0}\rangle = \prod_{\mathbf{k}\sigma} [1 + a^0_{\mathbf{k}\sigma} \hat{f}^+_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma}] |\,\mathrm{cFS}\rangle \tag{2}$$

where

$$a^0_{\mathbf{k}\sigma} = \frac{2V_{\mathbf{k}}}{\varepsilon^f_{\mathbf{k}} - \varepsilon^c_{\mathbf{k}} + \sqrt{(\varepsilon^c_{\mathbf{k}} - \varepsilon^f_{\mathbf{k}})^2 + 4V^2_{\mathbf{k}}}} \tag{3a}$$

and

$$|\,\mathrm{cFS}\rangle = \prod_{\substack{\mathbf{k},\sigma \\ \varepsilon^c_{\mathbf{k}} \le \varepsilon_F}} \hat{c}^+_{\mathbf{k}\sigma} |0\rangle \tag{3b}$$

is the Fermi sea of the conduction electrons, when all f-levels are unoccupied.

As first pointed out by Rice and Ueda[2] and Brandow[3] a *correlated* wave function for the PAM in the presence of interactions between the f-electrons may now be constructed in exact analogy with the Gutzwiller wave function for the Hubbard model.[4,5] Namely, a correlation operator parametrizing the f-electron on-site interaction is used as a project or acting on (2) to reduce the number of doubly occupied sites; this yields

$$|\Psi_{\mathrm{PAM}}(U)\rangle = g^{\hat{D}^f} |\Psi_{\mathrm{PAM},0}\rangle \tag{4}$$

where $0 \le g \le 1$ is a variational parameter and $\hat{D}^f = \sum_{\mathbf{i}} \hat{n}^f_{\mathbf{i}\uparrow} \hat{n}^f_{\mathbf{i}\downarrow}$ is the number operator of double f-occupancy. The choice of wave function is also inspired by the wave functions used in the investigations of the single-impurity model.[6,7] Since the number of f-electrons is not conserved, the suppression of double occupancy would favor the transfer of f-electrons into the conduction band, thus changing the effective hybridization. Therefore not only g, but also the function $a^0_{\mathbf{k}\sigma}$ in $|\Psi_0\rangle$, is used as a variational quantity to optimize $|\Psi_{\mathrm{PAM}}\rangle$, (4).

Within the Gutzwiller approximation[4] (corresponding to a semi-classical counting of spin configurations,[8] which becomes exactly in the limit of high dimensions[9–11] $d \to \infty$) the ground state energy of $\hat{H}_{\mathrm{PAM}}$ in terms of (4) is found as[2,12–14]

$$\frac{E^{\mathrm{Gutz}}_{\mathrm{PAM}}}{L} = -\frac{U}{2} + \varepsilon_0 - 2\exp\left(-\frac{U}{8V^2}\right) \tag{5}$$

where L is the number of lattice sites of the system. In (5) $V_{\mathbf{k}} \equiv V = \text{const}$, $\varepsilon^f_{\mathbf{k}} \equiv E_f = \text{const}$ and the symmetric case ($E_f = -U/2$) with $n = 2$ has been assumed. Furthermore $\varepsilon^c_{\mathbf{k}}$ was chosen to be linear, with $-1 \leq \varepsilon^c_{\mathbf{k}} \leq 1$, such that the average energy of the conduction electrons in the uncorrelated state, $\varepsilon_0 = (2/L) \sum_{\varepsilon^c_{\mathbf{k}} \leq 0} \varepsilon^c_{\mathbf{k}}$, is given by $\varepsilon_0 = -1/2$. The appearance of a non-analytic term in the ground state energy, i.e. of a binding energy having a Kondo form as in the *single-site* Kondo problem,[15] is remarkable. (In fact, the exponent differs by a factor 2 from the single site exponent; the appearance of this factor[16] has been shown to be a genuine *lattice* effect[17]). The result in (5), based on the Gutzwiller approximation, can also be derived by the *exact* evaluation of the ground state energy of the PAM in terms of (4) in the limit $d \to \infty$;[10,11,18] Other quantities, e.g. the momentum distribution and correlation functions, can be calculated analytically, too, in $d = \infty$ using the wave function. The limit $d = \infty$ may even be used to obtain information about the corresponding results for *finite* dimensions d (note that explicit analytic evaluations are no longer tractable in $d < \infty$). Indeed, we have recently shown[19,20] that, by evaluating the $d = \infty$ results with the d-dimensional density of states of the non-interacting system, one can obtain ***numerically*** correct results for the above quantities in the case of finite dimensions d. This even includes $d = 1$, where explicit comparison with variational Monte Carlo data[21] is possible. A similar conclusion was reached by Shiba and Fazekas[22] on the basis of their variational results for the ground state energy of the Kondo lattice in $d = 1$. According to these authors, the fact that the $d = \infty$ result obtained with (4) yields good results even in $d = 1$ is, at least in part, due to an approximation cancellation between an overestimation of the exchange energy and an underestimation of the conduction band energy at large U.

Sofar we have only shown that the d-dimensional ground state properties of the PAM, when calculated in terms of the wave functions (4), can be determined accurately down to $d = 1$ by employing the limits $d = \infty$. This does not address the point of how good the results obtained with (4) are in absolute terms, i.e. in comparison with the *exact* ground state wave function. In Fig. 1 the ground state energy of the PAM in $d = 1$ measured relative to $E_f = -\frac{U}{2}$, as obtained by means of the wave function (4), is shown (short-dashed line). It is compared with the results from numerical (Monte Carlo) calculations of Blankenbecler *et al.*[23] Obviously the wave function (4) yields good results only for *low* U, while at large U the energy is much higher than the exact result. The origin for this discrepancy at large U is easily found: it is mainly due to the absence of the (negative!) contribution to the energy from the second order perturbation theory in the hybridization V. Indeed, in the symmetric case and for large U perturbation theory in V yields[23,19,22]

$$\frac{E_{\mathrm{PAM}}^{\mathrm{exact}}}{L} = -\frac{U}{2} + \varepsilon_0 - \frac{2V^2}{L} \sum_{\substack{\mathbf{k} \\ \varepsilon_{\mathbf{k}}^c \geq 0}} \frac{1}{\frac{U}{2} + \varepsilon_{\mathbf{k}}^c} + \mathcal{O}(V^3) \tag{6a}$$

$$= -\frac{U}{2} + \varepsilon_0 - \frac{2V^2}{U}, \qquad U \gg |\varepsilon_0| \,. \tag{6b}$$

This result does not depend on the explicit configuration of f-electrons when double occupancy is excluded. In fact, the term $\propto -V^2/U$ is even present for a single f-spin and hence is not specific for the periodic model. Hence the second order shift in (6a) does not contain any information about the magnetic state of the system – this only comes in at higher order, i.e. V^4/U^2.[24,25] The same conclusion was reached by Shiba and Fazekas,[22] who showed that the second order contribution is automatically generated by a Schrieffer–Wolff transformation that leads from (1) to an effective Hamiltonian (the Kondo lattice with antiferromagnetic coupling).

The overall features of the result for the ground state energy of the PAM as obtained with the Gutzwiller-type wave function (4) are almost identical to those observed in the case of the Hubbard model.[5] Since the wave function introduces correlation into the *non-interacting* state, the energy comes out very well for weak interactions ($U \lesssim 3.2t$), but starts to deviate at larger values of U, where the wave function is no longer controlled by some exact limit. In both cases non-analytic contributions are obtained for large U. The fact that the wave function (4) for the PAM does not yield the second order shift $\propto -V^2/U$ (which is energetically important, but conceptually rather trivial) and only leads to a non-analytically small, Kondo-like energy contribution (which is energetically unimportant, but conceptually significant) raises the question about the reliability of this wave function. In particular, it is not clear whether the exponentially small energy shift in (5) is a genuine feature of the finite-dimensional lattice model (PAM) at all, or whether it is simply an artefact of the wave function (4), i.e. is a residual feature of the single-impurity model on which the construction of this wave function is based. In spite of some rather indirect indications supporting the Gutzwiller results,[26] this is still an open question at present.

3. The New Variational Wave Function

We will now present a new type of variational wave function which has two essential advantages over the Gutzwiller-type wave function (4): (i) evaluations can be performed analytically in arbitrary dimensions d and for arbitrary dispersions $\varepsilon_{\mathbf{k}}^c$, $\varepsilon_{\mathbf{k}}^f$, $V_{\mathbf{k}}$ and (ii) the second order shift $\propto -V^2/U$ in the ground state energy is correctly obtained in every dimension. In contrast to (4) the *correlations* will be mainly incorporated into the starting wave function, while the *hybridization* is introduced variationally be means of an operator. Our discussion will be limited to the symmetric case with $E_f = -U/2$ at half filling ($n = 2$, i.e. $n_f = n_c = 1$) on an A–B lattice with an *antiferromagnetically* ordered state of f-electrons. Indeed we

know from experiment[1] that there exist heavy fermion systems, e.g. YbP, U_2Zn_{17}, UCd_{11}, UCu_5, which exhibit antiferromagnetic order in the ground state. In these systems we do not expect Kondo-like exponential terms of the type discussed in the last section to be relevant. The variational wave function proposed by us has the form

$$|\Psi\rangle = \hat{C}|\Psi_0\rangle \tag{7a}$$

where the starting wave function $|\Psi_0\rangle$

$$|\Psi_0\rangle = |\mathrm{cFS}\rangle \otimes |\mathrm{Neél}\rangle \tag{7b}$$

is a product state of a Fermi sea of conduction electrons ($n_c = 1$) and a Neél state of localized f-electrons

$$|\mathrm{Neél}\rangle = \prod_{\substack{\mathbf{k},\sigma \\ \varepsilon_{\mathbf{k}}^c \le 0}} [\hat{f}_{\mathbf{k}\sigma}^+ + \sigma \hat{f}_{\mathbf{k}+\mathbf{Q}\sigma}^+]|0\rangle \,. \tag{8}$$

Here $\mathbf{Q} = (\pi, \pi, \ldots, \pi)$ is half a reciprocal lattice vector and $\varepsilon_{\mathbf{k}}^c + \varepsilon_{\mathbf{k}+\mathbf{Q}}^c = 0$. The correlator $\hat{C}$

$$\hat{C} = \exp\left(s \sum_{\mathbf{k}\sigma} [\hat{f}_{\mathbf{k}\sigma}^+ \hat{c}_{\mathbf{k}\sigma} + \hat{c}_{\mathbf{k}\sigma}^+ \hat{f}_{\mathbf{k}\sigma}]\right) \tag{9}$$

introduces the hybridization. The variational parameter s regulates the strength of hybridization between c- and f-electrons and is determined by the minimum of the ground state energy. The correlator (9) can be rewritten as

$$\hat{C} = \prod_{\mathbf{k}\sigma} \left[\sum_{m=0}^{\infty} \frac{1}{m!} s^m (\hat{f}_{\mathbf{k}\sigma}^+ \hat{c}_{\mathbf{k}\sigma} + \hat{c}_{\mathbf{k}\sigma}^+ \hat{f}_{\mathbf{k}\sigma})^m\right] \tag{10a}$$

$$= \prod_{\mathbf{k}\sigma} \left[1 + (\hat{f}_{\mathbf{k}\sigma}^+ \hat{c}_{\mathbf{k}\sigma} + \hat{c}_{\mathbf{k}\sigma}^+ \hat{f}_{\mathbf{k}\sigma}) \sinh s + (\hat{n}_{\mathbf{k}\sigma}^f - \hat{n}_{\mathbf{k}\sigma}^c)^2 (\cosh s - 1)\right] \,. \tag{10b}$$

Both $\hat{C}$ and the starting wave function $|\Psi_0\rangle$ in (7) are given by products over $\mathbf{k}$. Hence the (normalized) variational wave function can be written as a *product* wave function in $\mathbf{k}$-space.

$$|\Psi\rangle = \prod_{\substack{\mathbf{k},\sigma \\ \varepsilon_{\mathbf{k}}^c \le 0}} \frac{\hat{c}_{\mathbf{k}\sigma}^+ \hat{f}_{\mathbf{k}\sigma}^+ + \sigma(\sinh s \hat{f}_{\mathbf{k}\sigma}^+ + \cosh s \hat{c}_{\mathbf{k}\sigma}^+)(\cosh s \hat{f}_{\mathbf{k}+\mathbf{Q}\sigma}^+ + \sinh s \hat{c}_{\mathbf{k}+\mathbf{Q}\sigma}^+)}{\sqrt{1 + \cosh^2 2s}} |0\rangle \,. \tag{11}$$

This feature is in essential contrast to the Gutzwiller-type functions (cf. (4)); it will enable us to evaluate expectation values in terms of $|\Psi\rangle$ analytically in arbitrary dimensions d. For example, the momentum distribution of the f- and c-electrons are obtained as ($D(s)$: $= 1 + \cosh^2 2s$)

$$\langle \hat{n}_{\mathbf{k}\sigma}^f \rangle = \begin{cases} (1 + \sinh^2 s \cosh 2s)/D(s) & , \quad \varepsilon_{\mathbf{k}}^c < 0 \\ \cosh^2 s \cosh 2s/D(s) & , \quad \varepsilon_{\mathbf{k}}^c > 0 \end{cases} \tag{12a}$$

$$\langle \hat{n}^c_{\mathbf{k}\sigma} \rangle = \begin{cases} (1+\cosh^2 s \cosh 2s)/D(s) & , \quad \varepsilon^c_{\mathbf{k}} < 0 \\ \sinh^2 s \cosh 2s/D(s) & , \quad \varepsilon^c_{\mathbf{k}} > 0 \end{cases} \tag{12b}$$

$$\langle \hat{f}^+_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \rangle = \sinh 4s/4D(s), \text{ all } \mathbf{k} . \tag{12c}$$

Hence the f- and c-electron distributions are step functions with a discontinuity at $\mathbf{k} = \mathbf{Q}/2$. Note that the f-distribution increases at $\mathbf{k} = \mathbf{Q}/2$, while the c-distribution decreases. Furthermore, the double occupancy of f-eletrons is found as

$$\langle \hat{D}^f \rangle = \frac{1}{L} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \langle \hat{f}^+_{\mathbf{k}+\mathbf{q}\uparrow} \hat{f}_{\mathbf{k}\uparrow} \hat{f}^+_{\mathbf{k}'-\mathbf{q}\downarrow} \hat{f}_{\mathbf{k}'\downarrow} \rangle \tag{13a}$$

$$= L\left[\frac{1}{4} - \frac{\cosh^4 s}{[D(s)]^2}\right] . \tag{13b}$$

The results are valid in arbitrary dimensions d. For $\varepsilon^f_{\mathbf{k}} = E_f = -\frac{U}{2}$ and $V_k = V =$ const. the ground state energy of (1) is obtained as

$$\frac{E_{\mathrm{PAM}}}{L} = \frac{2\varepsilon_0 \cosh^2 s - V \sinh 4s}{1+\cosh^2 2s} - U\left[\frac{1}{4} + \frac{\cosh^4 s}{(1+\cosh^2 2s)^2}\right] . \tag{14}$$

Since small U corresponds to small s, the energy (14) is found in this limit as

$$\frac{E_{\mathrm{PAM}}}{L} = -\frac{U}{2} + \varepsilon_0 - 2Vs + \left(\frac{U}{2} - \varepsilon_0\right)s^2 \tag{15}$$

which after minimization with respect to s yields

$$\frac{E_{\mathrm{PAM}}}{L} = -\frac{U}{2} + \varepsilon_0 - \frac{V^2}{\frac{U}{2} - \varepsilon_0} . \tag{16}$$

Comparing (16) with the result from perturbation theory, (6a, b), shows that for $U \gg |\varepsilon_0|$ the variational wave function (11) indeed leads to the exact asymptotic result for the ground state energy, including the correct second order shift, in all dimensions. This was to be expected since (16) is a result of the starting wave function $|\Psi_0\rangle$ in (11) alone, where the f-electrons have no double occupancy (the antiferromagnetic order is unimportant here; see Sec. 2). The U-dependence of the ground state energy relative to E_f as obtained from (14) is also shown in Fig. 1 (full line). For large U the result is seen to coincide with the exact result obtained numerically.[23] Deviations only occur for $U \lesssim 3.2t$, i.e. outside the range of parameters for which the PAM was originally constructed.

4. Improvement of the New Variational Wave Function

Since $|\Psi\rangle$ in (11) is a product wave function in $\mathbf{k}$-space, improvements can easily be incorporated provided the product form is maintained. This is the case when

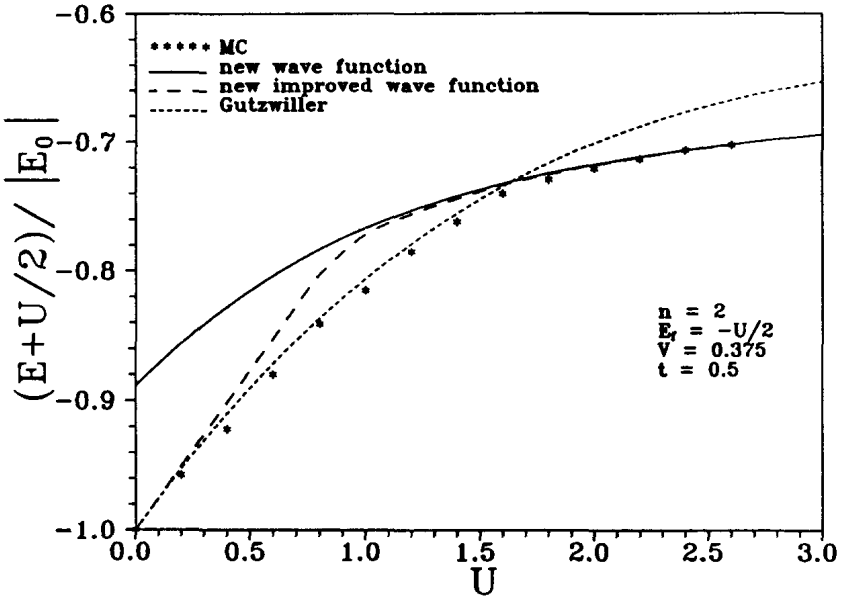

Fig. 1. Ground state energy E of the one-dimensional periodic Anderson model relative to the f-level $E_f = -U/2$ as a function of U; here $\varepsilon_k^c = -2t\cos k$. The results obtained with the new wave function, (7), (full line) and the improved version (see text; long-dashed line) are compared with those from the Gutzwiller wave function, (4) (short-dashed line) and exact Monte-Carlo results.[23]

additional, purely $\mathbf{k}$ dependent variational functions are introduced into $|\Psi\rangle$. Below we describe three possible improvements. Firstly, the starting wave function $|\Psi_0\rangle$, (7b), may be refined by replacing the rigid Neél state for the f-electrons by a Hartree–Fock wave function with antiferromagnetic long range order ("spin density wave" (SDW)):

$$|\text{Neél}\rangle \rightarrow |\text{SDW}\rangle = \prod_{\substack{\mathbf{k},\sigma \\ \varepsilon_{\mathbf{k}}^c \leq 0}} \left(u_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^{+} + \sigma v_{\mathbf{k}} \hat{f}_{\mathbf{k}+\mathbf{Q}\sigma}^{+}\right)|0\rangle \,. \tag{17a}$$

Secondly, the correlator $\hat{C}$ in (9) may be improved by allowing for a $\mathbf{k}$-dependence of the variational parameter s:

$$\hat{C} \rightarrow \hat{C}' = \exp\left(\sum_{\mathbf{k}\sigma} s_{\mathbf{k}} [\hat{f}_{\mathbf{k}\sigma}^{+} \hat{c}_{\mathbf{k}\sigma} + \hat{c}_{\mathbf{k}\sigma}^{+} \hat{f}_{\mathbf{k}\sigma}]\right) . \tag{17b}$$

For $u_{\mathbf{k}} = v_{\mathbf{k}} = s_{\mathbf{k}} = 1$ the wave function $|\Psi\rangle$ in (11) is reproduced. Thirdly, one may introduce an additional correlator $\hat{C}_1$

$$\hat{C}_1 = \exp\left(\sum_{\mathbf{k}\sigma} \tilde{\varepsilon}_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma}^{f}\right) \tag{17c}$$

which influences the hopping processes ("kinetic energy") of the f-electrons, with $\tilde{\varepsilon}_{\mathbf{k}}$ as a new $\mathbf{k}$-dependent variational function. The improved wave function then takes the form

$$|\Psi\rangle = \hat{C}_1 \hat{C}' |\mathrm{cFS}\rangle \otimes |\mathrm{SDW}\rangle \,. \tag{18a}$$

After normalization, we obtain

$$|\tilde{\Psi}\rangle = \prod_{\substack{\mathbf{k},\sigma \\ \epsilon^c_{\mathbf{k}} \le 0}} \left\{ \frac{1}{\sqrt{N_{\mathbf{k}}}} \left[e^{\tilde{\varepsilon}_{\mathbf{k}}} u_{\mathbf{k}} \hat{c}^+_{\mathbf{k}\sigma} \hat{f}^+_{\mathbf{k}\sigma} + \sigma v_{\mathbf{k}} \left(e^{\tilde{\varepsilon}_{\mathbf{k}}} \sinh s_{\mathbf{k}} \hat{f}^+_{\mathbf{k}\sigma} + \cosh s_{\mathbf{k}} \hat{c}^+_{\mathbf{k}\sigma} \right) \right. \right.$$

$$\left. \left. \times \left(e^{\tilde{\varepsilon}_{\mathbf{k}+\mathbf{Q}}} \cosh s_{\mathbf{k}+\mathbf{Q}} \hat{f}^+_{\mathbf{k}+\mathbf{Q}\sigma} + \sinh s_{\mathbf{k}+\mathbf{Q}} \hat{c}^+_{\mathbf{k}+\mathbf{Q}\sigma} \right) \right] \right\} |0\rangle \tag{18b}$$

where

$$N_{\mathbf{k}} = e^{2\tilde{\varepsilon}_{\mathbf{k}}} u^2_{\mathbf{k}} + v^2_{\mathbf{k}} \left(e^{2\tilde{\varepsilon}_{\mathbf{k}}} \sinh^2 s_{\mathbf{k}} + \cosh^2 s_{\mathbf{k}} \right) \left(e^{2\tilde{\varepsilon}_{\mathbf{k}+\mathbf{Q}}} \cosh^2 s_{\mathbf{k}+\mathbf{Q}} + \sinh^2 s_{\mathbf{k}+\mathbf{Q}} \right) . \tag{18c}$$

Here $\tilde{\varepsilon}_{\mathbf{k}}$, $s_{\mathbf{k}}$ and $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ with $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$ enter as variational functions. All expectation values in terms of $|\Psi\rangle$, e.g. of the momentum distributions and the double occupancy (cf. (12), (13)), can be calculated analytically.[19] It is interesting to note that – even without the improvements (17a), (17b) – the action of the new correlator $\hat{C}_1$, (17c), on $|\Psi\rangle$ in (11) guarantees the correct *low-U* dependence of the ground state energy of the PAM. This may be seen by taking the limit $u_{\mathbf{k}} = v_{\mathbf{k}} = 1$, $s_{\mathbf{k}} = s \to \infty$ in (18b), whereby

$$|\tilde{\Psi}\rangle \to - \prod_{\mathbf{k}\sigma} \frac{\hat{c}^+_{\mathbf{k}\sigma} + e^{\tilde{\varepsilon}_{\mathbf{k}}} \hat{f}^+_{\mathbf{k}\sigma}}{\sqrt{1 + e^{2\tilde{\varepsilon}_{\mathbf{k}}}}} |0\rangle \,. \tag{19}$$

Except for an unimportant phase factor this is identical with $|\Psi_{\mathrm{PAM},0}\rangle$, (2), i.e. the exact ground state wave function of the PAM for $U = 0$, with $\exp(\tilde{\varepsilon}_{\mathbf{k}}) = a^0_{\mathbf{k}\sigma}$. Hence the energy calculated with $|\Psi\rangle$ will not only yield the *large* U-behavior correctly but will even produce the correct linear term in U for *small* U. This behavior is shown in Fig. 1, where the long-dashed line represents the ground state energy for the PAM, (1), as obtained with $|\Psi\rangle$ in the case $V_{\mathbf{k}} = V$, $\varepsilon^f_{\mathbf{k}} = E_F = -U/2$, for the special choice $u_{\mathbf{k}} = v_{\mathbf{k}} = 1$, $s_{\mathbf{k}} = s$ and

$$\exp(\tilde{\varepsilon}_{\mathbf{k}}) = \frac{2Vr}{-\varepsilon^c_{\mathbf{k}} + \sqrt{(\varepsilon^c_{\mathbf{k}})^2 + 4V^2 r^2}} \,. \tag{20}$$

The parametrization in (20) is inspired by the form of $a^0_{\mathbf{k}\sigma}$, (3a); this leaves us with only two variational parameters (r and s) in the ground state energy, which, after minimization, leads to the curve shown in Fig. 1 (long-dashed line). There remains a deviation in the intermediate regime where $U \simeq 2t$. However, this part in parameter space can be controlled by a final improvement of the wave function, obtained by applying the *Gutzwiller correlator* to $|\tilde{\Psi}\rangle$:

$$|\Psi_{\mathrm{optim.}}\rangle = g^{\hat{D}'} |\tilde{\Psi}\rangle \,. \tag{21}$$

This wave function will always be better than the Gutzwiller-type wave function (4) (which leads to the correct low-U behavior (short-dashed line) up to $U/t \lesssim 3.2$) *and* the new wave function $|\tilde{\Psi}\rangle$ (which gives the correct large-U behavior (long-dashed line) for $U/t \gtrsim 3.2$). From Fig. 1 it is therefore clear that $|\Psi_{\text{optim.}}\rangle$, containing only three $\mathbf{k}$-independent variational parameters g, r, and s, will be an outstandingly good wave function (at least with respect to the energy) for the PAM. Due to the Gutzwiller correlator it is no longer analytically tractable. Evaluation should therefore employ variational Monte Carlo techniques. For arbitrary parameters $V_{\mathbf{k}}$, $\varepsilon^f_{\mathbf{k}}$ the variational functions $s_{\mathbf{k}}$, $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, $\tilde{\varepsilon}_{\mathbf{k}}$ must be parametrized by functions containing (few) $\mathbf{k}$-independent variational parameters since otherwise the minimization cannot be performed. In the case of $\varepsilon^f_{\mathbf{k}} = E_f - 2t' \sum_{n=1}^{d} \cos k_n$ the choice of a simple Hartree–Fock form for $u_{\mathbf{k}}$, $v_{\mathbf{k}}$

$$u_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left[1 + \sqrt{1 - \theta^2_{\mathbf{k}}} \right]^{\frac{1}{2}}$$

$$v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left[1 - \sqrt{1 - \theta^2_{\mathbf{k}}} \right]^{\frac{1}{2}}$$

with

$$\theta_k = \frac{\Delta}{\sqrt{(\varepsilon^f_{\mathbf{k}} - E_f)^2 + \Delta^2}} \,.$$

will be sufficient to obtain very good results for the ground state energy of the PAM for *all* values of U in *all* dimensions d.

5. Discussion

We have presented a new type of variational wave function for the periodic Anderson model. It applies to the symmetric case ($E_f = -U/2$) with $n = 2$ and assumes that anti-ferromagnetic long-range order of the f-electrons as is the case in some heavy fermion systems, such as UCu_5, U_2Zn_{17} etc. In contrast to the conventional Gutzwiller-type wave function the correlation of f-electrons is already mainly contained in the starting wave function and it is the hybridization between c- and f-electrons that is introduced by a variational procedure. This wave function has the advantage of being a product state in $\mathbf{k}$-space, which thereby allows for explicit analytic work in arbitrary dimensions d. Besides that it automatically leads to the correct contribution from second order perturbation theory in the hybridization V, $\propto -V^2/U$ for large U, which is systematically missing in the Gutzwiller approach. We have outlined further improvements of this wave function. In particular, the correct behavior of the energy at low U is then obtained, too. Application of an additional Gutzwiller projector for the f-electrons therefore provides one with a variational wave function that leads to excellent exact upper bounds for the ground state energies for the periodic Anderson model at arbitrary U in any dimension d.

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