# Exact Ground-State Energy of the Periodic Anderson Model in $d=1$ and Extended Emery Models in $d=1,2$ for Special Parameter Values

Rainer Strack

*Institut für Theoretische Physik C, Technische Hochschule Aachen, D-5100 Aachen, Federal Republic of Germany*

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We generalize an approach, which was recently introduced by Brandt and Giesekus to calculate the exact ground-state energy for strongly interacting particles on special perovskitelike lattices, to the periodic Anderson model in the dimension $d=1$ and to extended Emery models in $d=1,2$ on *regular* lattices for *arbitrary* spin degeneracy. For these models we calculate the exact ground-state energy for a restricted parameter regime in the strong-coupling limit. The ground-state energy shows a simple algebraic structure. We also present an eigenfunction of the Hamiltonian with the ground-state energy as its corresponding eigenvalue.

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The description of heavy fermion systems [1] by the periodic Anderson model [2] and of high-$T_c$ materials [3] by the Emery model [4] continues to attract considerable interest. Despite their simple structure exact results are rare. Recently, Brandt and Giesekus [5] introduced a new approach to calculate the exact ground-state energy for the Hubbard model and for a periodic Anderson model in the strong-coupling limit ($U=\infty$) on peculiar perovskitelike lattices. In addition, they presented an eigenfunction with the ground-state energy as the corresponding eigenvalue. In this paper we generalize their approach to the periodic Anderson model ($U=\infty$) with *arbitrary* spin degeneracy $N_\sigma$ in $d=1$ for a restricted, but reasonable, parameter regime at half filling. The exact ground-state energy thus obtained does not show a Kondo-like exponent. Furthermore, we calculate exactly the ground-state energy for extended Emery models [in $d=1$ we include an oxygen-oxygen hopping term and in $d=2$ a (rather artificial) copper-copper hopping term] in a restricted parameter regime for $U=\infty$ and for arbitrary spin degeneracy. Here $U$ refers to the on-site interaction term on the copper sites. In order to apply the procedure mentioned above we have to consider the Emery model in $d=1$ (CuO chains) in the particle picture and in $d=2$ ($CuO_2$ planes) in the hole picture. Whether at $U=\infty$ [6] the hole or the particle picture is the appropriate one, is not precisely clear [7].

*The periodic Anderson model in $d=1$.*—The Hamiltonian of the periodic Anderson model (PAM) in the strong-coupling limit is given by

$$\hat{H}_{\mathrm{PAM}}=\hat{P}\left\{\sum_{k,\sigma}[\epsilon_k^c\hat{n}_{k\sigma}^c+\epsilon_k^f\hat{n}_{k\sigma}^f+V_k(\hat{f}_{k\sigma}^\dagger\hat{c}_{k\sigma}+\hat{c}_{k\sigma}^\dagger\hat{f}_{k\sigma})]\right\}\hat{P}\,, \tag{1}$$

where $\hat{P}$ is a projector on the subspace of zero double occupancy of $f$ electrons, i.e., $\hat{P}=\prod_{i,\sigma\neq\sigma'}(1-\hat{n}_{i\sigma}^f\hat{n}_{i\sigma'}^f)$ with the combined spin and band index $\sigma=1,\ldots,N_\sigma$. Here, $\hat{c}_{k\sigma}^\dagger$ ($\hat{c}_{k\sigma}$) and $\hat{f}_{k\sigma}^\dagger$ ($\hat{f}_{k\sigma}$) create (destroy) a $c$ electron and an $f$ electron, respectively, with momentum $k$ and spin $\sigma$. The corresponding number operators are $\hat{n}_{k\sigma}^c=\hat{c}_{k\sigma}^\dagger\hat{c}_{k\sigma}$, $\hat{n}_{k\sigma}^f=\hat{f}_{k\sigma}^\dagger\hat{f}_{k\sigma}$. The index $i$ refers to a lattice site ($\hat{n}_{i\sigma}^f=\hat{f}_{i\sigma}^\dagger\hat{f}_{i\sigma}$, $\hat{n}_{i\sigma}^c=\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}$) with $\hat{f}_{i\sigma}^\dagger,\hat{c}_{i\sigma}^\dagger$ as the Fourier transforms of $\hat{f}_{k\sigma}^\dagger,\hat{c}_{k\sigma}^\dagger$. Within a tight-binding approximation the dispersion relations are given by $\epsilon_k^c=-2t\cos(k)$ and $\epsilon_k^f=E_f+2t'\cos(k)$ with $t,t'>0$. Note that we assume the sign of the $c$ electron dispersion to be different from that of the $f$ electron dispersion, because of the symmetry of the $c$ and $f$ orbitals. Because of that symmetry the hybridization matrix element $V_k$ has the form $V_k=2V\times\sin(k)$ (an on-site hybridization is forbidden because of parity reasons) [8].

In real space we define new operators

$$\hat{a}_{i\sigma}^\dagger=\frac{1}{\sqrt{2}}\left[\frac{i(\hat{f}_{i\sigma}^\dagger-\hat{f}_{i+1\sigma}^\dagger)}{(1+t^2/V^2)^{1/2}}-\frac{\hat{c}_{i\sigma}^\dagger+\hat{c}_{i+1\sigma}^\dagger}{(1+V^2/t^2)^{1/2}}\right], \tag{2}$$

which are not genuine Fermi operators [9]. In order to express the Hamiltonian $\hat{H}_{\mathrm{PAM}}$ in terms of these new operators $\hat{a}_{i\sigma}^\dagger$ we have to restrict the parameter regime to $t'=V^2/t$; thus we obtain

$$\hat{H}_{\mathrm{PAM}}=\hat{P}\left\{-2\left(t+\frac{V^2}{t}\right)\sum_{i,\sigma}\hat{a}_{i\sigma}^\dagger\hat{a}_{i\sigma}+L\left[\left(E_f+2\frac{V^2}{t}\right)\hat{n}_f+2t\hat{n}_c\right]\right\}\hat{P}\,, \tag{3}$$

with $\hat{n}_f=(1/L)\sum_{i\sigma}\hat{n}_{i\sigma}^f$, $\hat{n}_c=(1/L)\sum_{i\sigma}\hat{n}_{i\sigma}^c$, where $L$ is the number of lattice sites. The Hamiltonian can be further transformed by use of the following identities: $\hat{a}_{i\sigma}^\dagger\hat{a}_{i\sigma}=1-\hat{a}_{i\sigma}\hat{a}_{i\sigma}^\dagger$ and

$$\hat{P}\hat{a}_{i\sigma}\hat{a}_{i\sigma}^\dagger\hat{P}=\hat{a}_{i\sigma}\hat{P}\hat{a}_{i\sigma}^\dagger+\sum_{\sigma'(\neq\sigma)}(\hat{n}_{i\sigma'}^f+\hat{n}_{i+1\sigma'}^f)\hat{P}/(2+2t^2/V^2)\,.$$

In order to obtain an equation for $\hat{H}_{\mathrm{PAM}}$ where $\hat{n}=\hat{n}_f+\hat{n}_c$ enters we choose $E_f=2t-2N_\sigma V^2/t$. Hence, $\hat{H}_{\mathrm{PAM}}$ may be written as

$$\hat{H}_{\mathrm{PAM}} = \left[ -2N_\sigma \left( t + \frac{V^2}{t} \right) + 2t\hat{n} \right] \hat{P} L + 2\left( t + \frac{V^2}{t} \right) \sum_{i,\sigma} \hat{\alpha}_{i\sigma} \hat{P} \hat{\alpha}^\dagger_{i\sigma} . \quad (4)$$

No approximation has been made. Equation (4) is an exact expression for $\hat{H}_{\mathrm{PAM}}$ in the case of $t' = V^2/t$, $E_f = 2t - 2N_\sigma V^2/t$. Since $\hat{\alpha}_{i\sigma}\hat{P}\hat{\alpha}^\dagger_{i\sigma}$ is positive semidefinite ($\hat{P}^2 = \hat{P}$) we have found a lower bound $E_l = [-2N_\sigma(t + V^2/t) + 2tn]L$ of the exact ground-state energy $E_0$, where $n$ is the eigenvalue of $\hat{n}$. In order to obtain an upper bound we consider the wave function

$$|\Psi\rangle = \hat{P} \prod_{i,\sigma} \hat{\alpha}^\dagger_{i\sigma} |0\rangle , \quad (5)$$

where $|0\rangle$ is the vacuum state. This wave function corresponds to a total density $n = N_\sigma$. One can easily verify that $|\Psi\rangle$ is an eigenfunction of $\hat{H}_{\mathrm{PAM}}$ with the eigenvalue $E_u = -(2N_\sigma V^2/t)L$. From the variational principle it follows that $E_u$ is an upper bound of the ground-state energy. Since the upper and the lower bound coincide for $n = N_\sigma$, the exact ground-state energy for the periodic Anderson model in $d = 1$ is given by

$$E_0 = -(2N_\sigma V^2/t)L , \quad (6)$$

where we set $t' = V^2/t$, $E_f = 2t - 2N_\sigma V^2/t$, and $n = N_\sigma$. In other words we have calculated the ground-state energy for the following dispersion relation of the $f$ electrons: $\epsilon^f_k = 2t - (2N_\sigma V^2/t) + (2V^2/t)\cos(k)$. The choice $N_\sigma = 8$, $t = 1$ eV, $V = 0.4$ eV, $E_f = -0.56$ eV, and $t' = 0.16$ eV which fulfills the two parameter constraints yields values which are within the expected range.

It is a remarkable fact that the ground-state energy has such a simple algebraic structure. There is no Kondo-like exponent in the energy. This Kondo term has been predicted by several approximation schemes, such as the mean-field approximation (slave bosons) [10] or the Gutzwiller approximation [11,12]. In these theories the single-impurity exponent survives also in the lattice case with a slight modification. Obviously, in the one-dimensional periodic Anderson model this Kondo-like exponent does not exist on the hypersurface of parameter values that is determined by $t' = V^2/t$, $E_f = 2t - 2N_\sigma V^2/t$. It is possible that the parameter restriction is responsible for the disappearance of this term [13]. In addition, we present a *nonmagnetic* eigenfunction [see (5)] of the Hamiltonian with the ground-state energy as its corresponding eigenvalue. We cannot decide if this energy is degenerate. The eigenfunction is of the Gutzwiller type, because $\hat{P}$ is the Gutzwiller correlator for $U = \infty$ and $\prod_{i,\sigma} \hat{\alpha}^\dagger_{i\sigma}|0\rangle$ is the ground-state wave function for the uncorrelated system ($U = 0$) [but for a different $E_f$ value $E_f^{(U=0)} = E_f^{(U=\infty)} + 2(N_\sigma - 1)V^2/t$] [11,12,14]. Such a characteristic of the eigenfunction was already found by Brandt and Giesekus [5] on perovskitelike lattices.

*The extended Emery model in $d = 1$.*—The Emery model describes strongly interacting particles (holes) on a two-dimensional lattice [4]. For reasons of simplicity one often considers this model in $d = 1$ [15]. Hence, we first investigate the model on a CuO chain ($d = 1$). In order to apply the approach presented above we include a hopping term between O sites, which is a reasonable extension of the Emery model. The Hamiltonian under investigation is given by

$$\hat{H}^{(1)}_E = \hat{P} \left[ V \sum_{i,\sigma} [\hat{d}^\dagger_{i\sigma}(\hat{p}_{i+a\sigma} - \hat{p}_{i-a\sigma}) + \mathrm{H.c.}] + t \sum_{i,\sigma} (\hat{p}^\dagger_{i+a\sigma}\hat{p}_{i-a\sigma} + \mathrm{H.c.}) + \epsilon_d \sum_{i,\sigma} \hat{n}^d_{i\sigma} + \epsilon_p \sum_{i,\sigma} \hat{n}^p_{i+a\sigma} \right] \hat{P} \quad (7)$$

in the strong correlated limit (particle picture). The lattice consists of alternate copper and oxygen atoms. The parameter $i$ runs over the Cu sites and $i \pm a$ refers to the neighboring O sites, where $a$ is half the distance between two Cu sites. The operator $\hat{d}^\dagger_{i\sigma}$ ($\hat{p}^\dagger_{i+a\sigma}$) creates a particle with spin $\sigma$ ($\sigma = 1, \ldots, N_\sigma$) on the Cu (O) site. The corresponding number operators are $\hat{n}^d_{i\sigma}$ ($\hat{n}^p_{i+a\sigma}$). Here, $V$ parametrizes the hopping between a Cu site and the neighboring O sites (we take the phase of the orbitals into account) and $t > 0$ is the hopping integral between O sites. The parameter for the local energy of the $d$ ($p$) particles is defined by $\epsilon_d$ ($\epsilon_p$). Furthermore, $\hat{P}$ is the projector on the subspace of zero double occupancy on Cu sites.

The procedure for determining the exact ground-state energy is nearly the same as above. First of all we define new operators (no genuine Fermi operators)

$$\hat{\alpha}^\dagger_{i\sigma} = \frac{1}{(1 + 2t^2/V^2)^{1/2}} \left\{ \left[ \hat{d}^\dagger_{i\sigma} - \frac{t}{V}(\hat{p}^\dagger_{i+a\sigma} - \hat{p}^\dagger_{i-a\sigma}) \right] \right\} . \quad (8)$$

As for the PAM we transform the Hamiltonian in terms of these new operators, where we restrict the calculation to the parameter regime

$$\epsilon_d + N_\sigma V^2/t = \epsilon_p + 2t . \quad (9)$$

With $\hat{n} = (1/L)\sum_{i,\sigma}(\hat{n}^d_{i\sigma} + \hat{n}^p_{i+a\sigma})$, where $L$ is the number of Cu sites, the transformed Hamiltonian may be written as

$$\hat{H}^{(1)}_E = \left[ -N_\sigma \left( 2t + \frac{V^2}{t} \right) + (\epsilon_p + 2t)\hat{n} \right] \hat{P} L + \left( 2t + \frac{V^2}{t} \right) \sum_{i,\sigma} \hat{\alpha}_{i\sigma} \hat{P} \hat{\alpha}^\dagger_{i\sigma} . \quad (10)$$

By means of the discussion presented above the exact ground-state energy $E_0$ for $n = N_\sigma$ is given by

$$E_0 = N_\sigma(\epsilon_p - V^2/t)L , \quad (11)$$

where we set $\epsilon_d+N_\sigma V^2/t=\epsilon_p+2t$. Usually, one considers $N_\sigma=2$ ($\sigma=\uparrow,\downarrow$). In this case the corresponding eigenfunction $|\Psi\rangle=\hat{P}\prod_{i,\sigma}\hat{a}^\dagger_{i\sigma}|0\rangle$ has the explicit form

$$|\Psi\rangle=\prod_i\left[\frac{t/V}{1+2t^2/V^2}\left(\frac{t}{V}(\hat{p}^\dagger_{i+a\uparrow}-\hat{p}^\dagger_{i-a\uparrow})(\hat{p}^\dagger_{i+a\downarrow}-\hat{p}^\dagger_{i-a\downarrow})+\hat{d}^\dagger_{i\downarrow}(\hat{p}^\dagger_{i+a\uparrow}-\hat{p}^\dagger_{i-a\uparrow})-\hat{d}^\dagger_{i\uparrow}(\hat{p}^\dagger_{i+a\downarrow}-\hat{p}^\dagger_{i-a\downarrow})\right)\right]|0\rangle\,, \qquad (12)$$

and it is obviously *nonmagnetic*. Locally, this wave function consists of a superposition of a Zhang-Rice-like singlet [16] $\hat{d}^\dagger_{i\downarrow}(\hat{p}^\dagger_{i+a\uparrow}-\hat{p}^\dagger_{i-a\uparrow})-\hat{d}^\dagger_{i\uparrow}(\hat{p}^\dagger_{i+a\downarrow}-\hat{p}^\dagger_{i-a\downarrow})$ and a term $(\hat{p}^\dagger_{i+a\uparrow}-\hat{p}^\dagger_{i-a\uparrow})(\hat{p}^\dagger_{i+a\downarrow}-\hat{p}^\dagger_{i-a\downarrow})$. As in the case of the PAM we do not know if the ground state is degenerate. The same model (only in the hole representation) for $N_\sigma=2$ was investigated by means of a mean-field approximation (slave bosons) by Grilli, Kotliar, and Millis [17]. They obtained a Kondo-like behavior of the ground state as for the PAM. We showed by our *exact* result that such a term does not exist in the parameter regime defined by Eq. (9). The exact ground-state energy has a very simple, algebraic structure, there is no nonanalyticity. In high-$T_c$ materials one expects $t<V$, $\epsilon_d>\epsilon_p$ (particle picture). Here we investigated the opposite case [take $t<V$ then $\epsilon_d<\epsilon_p$ from (9) for $N_\sigma=2$]. Nevertheless, this exact energy (11) and the corresponding eigenfunction (12) provide certain insight into the ground-state properties of the Emery model in $d=1$ for a parameter regime which is restricted only by a single equation [see (9)].

*The extended Emery model in $d=2$.*—We investigate the ground-state properties of the Emery model on a two-dimensional $CuO_2$ lattice. Instead of the O-O hopping we include a hopping term between Cu sites. We can deduce the exact ground-state energy only with this assumption [18]. This additional hopping may be described by a parameter $t$, which is small in comparison with the Cu-O hybridization. It is necessary for our calculation to consider this model in the hole picture. Hence, the Hamiltonian is given by

$$\hat{H}_E^{(2)}=\hat{P}\left[\sum_{\langle\mathbf{i},\mathbf{j}\rangle,\sigma}V_{\mathbf{ij}}(\hat{d}^\dagger_{\mathbf{i}\sigma}\hat{p}_{\mathbf{j}\sigma}+\mathrm{H.c.})+t\sum_{\langle\mathbf{ii'}\rangle,\sigma}(\hat{d}^\dagger_{\mathbf{i}\sigma}\hat{d}_{\mathbf{i'}\sigma}+\mathrm{H.c.})+\epsilon_d\sum_{\mathbf{i},\sigma}\hat{n}^d_{\mathbf{i}\sigma}+\epsilon_p\sum_{\mathbf{j},\sigma}\hat{n}^p_{\mathbf{j}\sigma}\right]\hat{P} \qquad (13)$$

in the strong correlated limit. Here, $\mathbf{i},\mathbf{i'}$ run over the Cu sites and $\mathbf{j}$ over the O sites. The index $\langle\cdots\rangle$ stands for summation over nearest neighbors. The operator $\hat{d}^\dagger_{\mathbf{i}\sigma}$ ($\hat{p}^\dagger_{\mathbf{j}\sigma}$) creates a hole with spin $\sigma$ on the Cu (O) site. The corresponding number operators are $\hat{n}^d_{\mathbf{i}\sigma}$ ($\hat{n}^p_{\mathbf{j}\sigma}$). Here, $V_{\mathbf{ij}}$ parametrizes the hopping between a Cu site and its neighboring O sites and is given by

$$V_{\mathbf{ij}}=\begin{cases}V \text{ for } \mathbf{j}=\mathbf{i}-\frac{1}{2}\mathbf{y} \text{ or } \mathbf{j}=\mathbf{i}-\frac{1}{2}\mathbf{x}\,,\\ -V \text{ for } \mathbf{j}=\mathbf{i}+\frac{1}{2}\mathbf{y} \text{ or } \mathbf{j}=\mathbf{i}+\frac{1}{2}\mathbf{x}\,,\end{cases} \qquad (14)$$

where $\mathbf{x},\mathbf{y}$ are unit vectors in the $x,y$ direction. As in the one-dimensional case we take the phase of the orbitals into account. The hopping integral between Cu sites is given by $t>0$. The parameter for the local energy of the $d$ ($p$) hole is defined by $\epsilon_d$ ($\epsilon_p$). Note that these energies are different from the ones above because here we consider the hole picture. Furthermore, $\hat{P}$ is the projector on the subspace of zero double occupancy on Cu sites.

As in the previous models we define new operators (no genuine Fermi operators)

$$\hat{a}^\dagger_{\mathbf{j}\sigma}=\frac{1}{(1+2t^2/V^2)^{1/2}}\left\{\left[\hat{p}^\dagger_{\mathbf{j}\sigma}-\frac{t}{V}(d^\dagger_{\mathbf{j}1\sigma}-\hat{d}^\dagger_{\mathbf{j}2\sigma})\right]\right\}, \qquad (15)$$

where $\mathbf{j}1$, $\mathbf{j}2$ are the neighboring Cu sites of the O site $\mathbf{j}$. We restrict the calculation to the parameter regime

$$\epsilon_d+4N_\sigma t=\epsilon_p+V^2/t\,. \qquad (16)$$

The transformed Hamiltonian has the final form

$$\hat{H}_E^{(2)}=\left[-2N_\sigma\left(2t+\frac{V^2}{t}\right)+\left(\epsilon_p+\frac{V^2}{t}\right)\hat{n}\right]\hat{P}L+\left(2t+\frac{V^2}{t}\right)\sum_{\mathbf{j},\sigma}\hat{a}_{\mathbf{j}\sigma}\hat{P}\hat{a}^\dagger_{\mathbf{j}\sigma} \qquad (17)$$

with $\hat{n}=(1/L)(\sum_{\mathbf{i},\sigma}\hat{n}^d_{\mathbf{i}\sigma}+\sum_{\mathbf{j},\sigma}\hat{n}^p_{\mathbf{j}\sigma})$, where $L$ is the number of Cu sites. From this expression it follows (see the previous sections) that the exact ground-state energy for $n=2N_\sigma$ is given by

$$E_0=2N_\sigma(\epsilon_p-2t)L\,, \qquad (18)$$

where we set $\epsilon_d+4N_\sigma t=\epsilon_p+V^2/t$. The corresponding eigenfunction $|\Psi\rangle=\hat{P}\prod_{\mathbf{j},\sigma}\hat{a}^\dagger_{\mathbf{j}\sigma}|0\rangle$ is *nonmagnetic*. As mentioned above we do not know if the ground state is degenerate. In high-$T_c$ materials one expects $t\ll V$, $\epsilon_d<\epsilon_p$ (hole picture). For $N_\sigma=2$ the choice $V=1$ eV, $t=0.4$ eV, and $\epsilon_p-\epsilon_d=0.7$ eV which fulfills Eq. (16) lies at the edge of the physically reasonable regime for high-$T_c$ materials. Usually one assumes that the direct hopping between Cu sites can be neglected. For very small $t$ Eq. (16) is only fulfilled for $\epsilon_d>\epsilon_p$ which is an unphysical parameter regime. This approach to the two-dimensional Emery model can be generalized also to higher dimensions.

In this paper we calculated the *exact* ground-state energies for the periodic Anderson model in $d=1$ and extended Emery models in $d=1,2$ in the strong correlated limit for a fixed density of particles (holes) and for arbitrary spin degeneracy $N_\sigma$. We presented the exact energies, which show very simple algebraic structure, for a restricted parameter regime. In the case of the PAM we do not find a Kondo-like exponent in the exact ground-state energy for all $N_\sigma$. Additionally, we presented *nonmagnetic* eigenfunctions with the ground-state energies as their corresponding eigenvalues. The one-dimensional results cannot be generalized to higher dimensions in contrast to the models investigated by Brandt and Giesekus [5]. These exact results may be used as a benchmark for Monte Carlo studies of the periodic Anderson model in $d=1$ and of the Emery model in $d=1,2$.

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