Hubbard and Anderson Models on Perovskitelike Lattices: Exactly Solvable Cases

Uwe Brandt and Andreas Giesekus
Institut für Physik, Universität Dortmund, Postfach 500 500, D-4600 Dortmund 50, Germany
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Exact solutions of the Hubbard model and the periodic Anderson model in the limit of infinite interaction strength are presented. Both models are studied on a D-dimensional decorated hypercubic lattice with periodic boundary conditions for any dimension $D \geq 2$ and arbitrary size. The lattice is very similar to the perovskite lattice. In addition to the ground-state energy, a corresponding eigenstate is constructed. This ground state contains at least two particles per unit cell. For the Anderson model, the exact solution is restricted to a surface in the (E_f, V) parameter space; however, the resulting relation $V(E_f)$ does not lead to unphysical parameters.

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Strongly interacting many-particle systems are a classical problem in solid-state physics. Numerous experiments indicate the breakdown of one-particle pictures; however, the theoretical description of truly interacting systems is far from being satisfactory. Highly correlated Fermi systems are frequently modeled by the familiar Hubbard and Anderson Hamilton operators [1]. These models describe the interplay between properties of itinerant and strongly interacting electrons; however, they only contain the absolute minimum of "ingredients" in order to remain tractable. Unfortunately, these models are still very complicated and exact results [2] are rare. In the light of this situation, it is highly valuable to obtain additional exact results as constraints for approximation schemes.

The model Hamiltonians and a particular D-dimensional lattice are defined. For these systems, the ground-state energy and a corresponding eigenstate are calculated analytically in the limit of infinite interaction strength $(U \to \infty)$ for any dimension $D \geq 2$. In a first step, the model Hamiltonians are rewritten in terms of suitable operators. This operator transformation is surprisingly simple, and the eigenstate which is an exact ground state follows immediately. In order to discuss the nature of the ground state in the final part of this Letter, the one-particle spectra of the models are briefly mentioned.

The lattice.—The exact solution of the Hubbard and Anderson models is an unsolved problem; however, a particular lattice where a solution is obtained may be derived from a D-dimensional decorated cubic lattice: The cubic lattice vectors are denoted by R, and the D basis vectors by e_ν. The electronic orbitals are located at the "decorated" sites $r = R + \frac{1}{2} e_\nu$, i.e., at the centers of the cubic bonds. The unit cell of this lattice $\mathcal{U}(R)$ contains D sites. For the sake of brevity, the set of all 2D sites $r = R \pm \frac{1}{2} e_\nu$ surrounding a lattice point R is called $\mathcal{N}(R)$. Figure 1 illustrates this lattice for $D = 2$. The cubic lattice points are represented by open circles, and the particle sites by solid circles, respectively.

For $D = 3$ the sites $\mathcal{N}(R)$ form octahedra. The structure of such a lattice is similar to the ReO_3 structure. (It is possible to consider the number of unit cells in one of the three dimensions to be 1, a lattice realized in the Cu-O planes including the apex oxygen atoms in high-T_c materials.)

Hopping.—Hopping is allowed between nearest-neighbor sites (along the edges) *and* those next-nearest-neighbor sites that are connected across the center of a D-dimensional octahedron. The approach introduced here requires that both types of hopping have the same matrix element $-t$ (with *positive* t). Figure 1 illustrates the hopping by solid lines, connecting solid circles. Periodic boundary conditions are assumed. The kinetic energy term of the model Hamiltonians (for spin σ) then reads

$$\mathbf{T}_\sigma = -t \sum_R \sum_{r \neq r' \in \mathcal{N}(R)} c^\dagger_{r,\sigma} c_{r',\sigma} , \tag{1}$$

where the operators $c^\dagger_{r,\sigma}$ ($c_{r,\sigma}$) create (annihilate) particles at the site r with spin σ. They obey Fermi statistics.

Hubbard model.—The Hubbard model is studied in the limit of infinite interaction strength. This simply excludes double occupancy of orbitals at the same lattice site, i.e., the interaction reduces the Hilbert space of the Hamilton operator to those states where the occupation number at any site r does not exceed 1. The operator $\mathbf{P}_H = \prod_r (1 - c^\dagger_{r,\uparrow} c_{r,\uparrow} c^\dagger_{r,\downarrow} c_{r,\downarrow})$ projects onto this subspace.

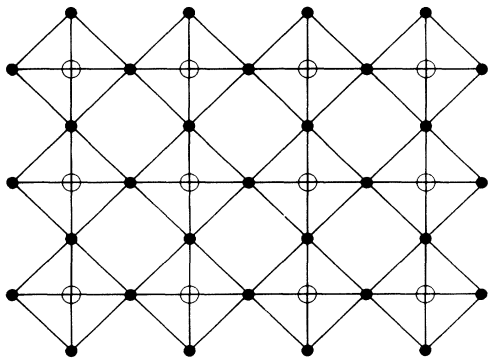

FIG. 1. Two-dimensional illustration of the lattice. The hopping matrix elements t are indicated by solid lines connecting solid circles.

The Hubbard Hamiltonian $\mathbf{H}_H$ for the case considered here is most conveniently written as

$$\mathbf{H}_H = \mathbf{P}_H \left(\sum_\sigma \mathbf{T}_\sigma \right) \mathbf{P}_H . \tag{2}$$

Note that this model contains just the parameter t, which defines the energy scale only.

Anderson model.—The Anderson model describes the interplay between electrons in extended orbitals (itinerant electrons), where the Coulomb interaction plays a minor role, and electrons in localized states, where the Coulomb interaction is the dominant influence on the electronic behavior. The Anderson model studied here is defined on the lattice described above. The itinerant electrons are described by the hopping Hamiltonian Eq. (1). The localized orbitals are placed at the cubic lattice points R (at the center of the hyperoctahedra). They have an on-site energy

$$\mathbf{H}_{f,\sigma} = E_f \sum_R f^\dagger_{R,\sigma} f_{R,\sigma} , \tag{3}$$

and the effect of hybridization between the itinerant and localized particles is incorporated by the usual hybridization term

$$\mathbf{H}_{cf,\sigma} = V \sum_R \sum_{r \in \mathcal{N}(R)} (f^\dagger_{R,\sigma} c_{r,\sigma} + \text{H.c.}) . \tag{4}$$

The interaction in this model affects the localized orbitals only and is described analogously by a projection operator $\mathbf{P}_A$ excluding f-orbital double occupancy. The Hamiltonian $\mathbf{H}_A$,

$$\mathbf{H}_A(E_f, V) = \mathbf{P}_A \sum_\sigma (\mathbf{T}_\sigma + \mathbf{H}_{f,\sigma} + \mathbf{H}_{cf,\sigma}) \mathbf{P}_A , \tag{5}$$

is solved below. Only the parameters E_f and V are chosen as independent parameters, t is considered to define the energy scale.

Solution of the Hubbard model.—The Hubbard model as defined above can be solved by means of a rather simple operator transformation. This transformation is based on the linear combination

$$\psi^\dagger_{R,\sigma} = (2D)^{-1/2} \sum_{r \in \mathcal{N}(R)} c^\dagger_{r,\sigma} \tag{6}$$

which generates a uniform distribution of electrons in the neighborhood $\mathcal{N}(R)$ of the lattice point R. Note that these new operators do not fully obey Fermi commutation rules:

$$[\psi^\dagger_{R,\sigma}, \psi_{R',\sigma'}]_+ = \delta_{\sigma,\sigma'} \begin{cases} 1, & \text{if } R = R', \\ (2D)^{-1}, & \text{if } R, R' \text{ nn}, \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

Nevertheless they are useful, because the expression $\sum_R \psi^\dagger_{R,\sigma} \psi_{R,\sigma}$ contains the kinetic energy operator (1) and the particle number operator. By using the identity $[c^\dagger_{r,\sigma}, \mathbf{P}_H]_- = c^\dagger_{r,-\sigma} c_{r,-\sigma} c^\dagger_{r,\sigma} \mathbf{P}_H$ the Hubbard Hamiltonian Eq. (2) may be written in terms of these new operators in the pseudodiagonal representation,

$$\mathbf{H}_H = -4t \mathbf{P}_H (DN - \mathbf{N}_c) \mathbf{P}_H + \mathbf{R} , \tag{8}$$

where the operator $\mathbf{N}_c = \sum_{r,\sigma} c^\dagger_{r,\sigma} c_{r,\sigma}$ denotes the particle number and $\mathbf{R}$ is defined as

$$\mathbf{R} = 2Dt \sum_{R,\sigma} \psi_{R,\sigma} \mathbf{P}_H \psi^\dagger_{R,\sigma} . \tag{9}$$

It is emphasized that the representation (8) of $\mathbf{H}_H$ is an operator *identity*; no approximations are applied. The essential advantage of this representation is the following: The Hamiltonian $\mathbf{H}_H$ is written in terms of a c number $(-4DtN)$, an operator that commutes with the Hamiltonian $(-4t\mathbf{N}_c)$, and a positive semidefinite remainder, the operator $\mathbf{R}$. It follows immediately that the ground-state energy $\mathcal{E}_H$ for this system may be estimated from below by

$$\mathcal{E}_H \geq -4t(DN - N_c) . \tag{10}$$

N_c is the eigenvalue of the particle number operator $\mathbf{N}_c$. This inequality is valid for any particle number N_c, dimension D, and number of unit cells N.

In the following, an eigenstate of $\mathbf{H}_H$ is derived and it will be shown that inequality (10) is fulfilled as an equality: Consider the projected state

$$|\psi\rangle = \mathbf{P}_H |\psi_0\rangle \text{ with } |\psi_0\rangle = \left(\prod_{R,\sigma} \psi^\dagger_{R,\sigma} \right) |\chi\rangle . \tag{11}$$

If $|\chi\rangle$ denotes the vacuum state, the state $|\psi\rangle$ contains two particles per unit cell. The norm of $|\psi_0\rangle$ does not vanish if *one* of the D system lengths equals an odd number of unit cells. The projected state $|\psi\rangle$ does not vanish, because its scalar product with a trial state $|\phi\rangle = \prod_R c^\dagger_{r,\uparrow} c^\dagger_{r',\downarrow} |\chi\rangle$ is nonzero, if *two* of the D system lengths are odd. [The sites r and r' are located at bonds in the directions $e_\mu \neq e_\nu$ within the same unit cell $\mathcal{U}(R)$. The restriction on the system lengths results from our choice of the trial state. It is not necessary; however, it is sufficient.]

Because of the operator identity $\mathbf{P}_H \psi^\dagger_{R,\sigma} \mathbf{P}_H \psi^\dagger_{R,\sigma} = 0$ the only nontrivial term in the eigenvalue equation, $\mathbf{R}|\psi\rangle$, vanishes. Consequently, the state $|\psi\rangle$ is an eigenstate of $\mathbf{H}_H$ and the inequality

$$\mathcal{E}_H \leq \langle \psi | \mathbf{H}_H | \psi \rangle = -4t(DN - N_c) \tag{12}$$

holds. The upper bound on the ground-state energy Eq. (12) and the lower bound Eq. (10) coincide.

The method presented here requires particle numbers larger than $2N$. The Hubbard system under consideration contains DN sites. Consequently, the two-dimensional case represents a half-filled system, and nontrivial results are only obtained for $D \geq 3$.

The inequalities (10) and (12) remain valid if the state $|\chi\rangle$ contains additional particles. It is possible to construct such states explicitly and it may be shown that their norm does not vanish. The discussion of this gen-

eralization will be published elsewhere.

Solution of the Anderson model.—The periodic Anderson model as introduced above may be treated in a completely analogous manner. The generalized operators

$$\psi^{\dagger}_{R,\sigma}=\alpha\left[(2D)^{-1/2}\sum_{r\in\mathcal{N}(R)}c^{\dagger}_{r,\sigma}\right]+\beta f^{\dagger}_{R,\sigma} \tag{13}$$

(with $|\alpha|^2+|\beta|^2=1$) allow us to obtain the following identity:

$$\mathbf{P}_A\sum_{\sigma}\left[T_\sigma-\frac{2Dt\lambda}{E_f}\left(\frac{\beta}{\alpha}\right)^2\mathbf{H}_{f,\sigma}-\frac{\sqrt{2D}\,t}{V}\frac{\beta}{\alpha}\mathbf{H}_{cf,\sigma}\right]\mathbf{P}_A$$
$$=\frac{2Dt}{\alpha^2}\sum_{R,\sigma}\psi_{R,\sigma}\mathbf{P}_A\psi^{\dagger}_{R,\sigma}-\mathbf{P}_A\left\{\frac{4DtN}{\alpha^2}-2t\left[\mathbf{N}_c+(2-\lambda)D\left(\frac{\beta}{\alpha}\right)^2\mathbf{N}_f\right]\right\}\mathbf{P}_A\,. \tag{14}$$

In contrast to the Hubbard case, an immediate identification of the Anderson Hamilton operator in the expression above is not possible, unless the coefficients of $\mathbf{H}_{f,\sigma}$ and $\mathbf{H}_{cf,\sigma}$ [3] on the left-hand side of Eq. (14) become identical to -1. Further, it is necessary that the combination of occupation-number operators on the right-hand side of Eq. (14) add up to the *conserved* quantity $\mathbf{N}_c+\mathbf{N}_f$. The conditions result in a restriction of the parameter space, because the number of equations exceeds the number of freely adjustable parameters. The solution of the resulting simple system of equations requires that V and E_f obey

$$V^2=t^2-\tfrac{1}{2}tE_f\,, \tag{15}$$

and, as a consequence, E_f must be smaller than $2t$. The ground-state energy $\mathcal{E}_A$ of the Hamiltonian Eq. (5) is obtained by the same arguments as presented for the Hubbard case:

$$\mathcal{E}_A=2tN_e-4DtN/\alpha^2\,, \tag{16}$$

$$1/\alpha^2=1+(2t-E_f)/4Dt\,, \tag{17}$$

where N_e denotes the total electron number. Similar to the above discussion, $N_e\geq 2N$ must be fulfilled, otherwise Eq. (16) just becomes a lower bound on the ground-state energy. In contrast to the Hubbard model, the case $D=2$ for the periodic Anderson model does not represent half filling.

It would be desirable to avoid the restriction of the (E_f,V) parameter space. However, this surface Eq. (15) is at least partially located in a regime of phenomenologically relevant parameters. (The resulting magnitude of the hybridization V may be somewhat large.)

One-particle properties.—Before the results of the previous section are further analyzed, the properties of the noninteracting system are briefly introduced. The band structure and the corresponding Bloch states allow at least some analysis of the eigenstates calculated above. Spin indices are omitted where not needed.

Hubbard case.—The band structure of the hopping system consists of one dispersive shifted tight-binding band

$$\epsilon(k)=2t[1-\epsilon_{\mathrm{tb}}(k)]\,, \tag{18}$$

where $\epsilon_{\mathrm{tb}}(k):=D+\sum_\mu\cos(k_\mu)$. The $D-1$ remaining "bands" form degenerate k-independent atomic states located at the upper band edge with energy $\epsilon=2t$.

Anderson case.—The one-particle spectrum of the Anderson model is slightly more complicated, because there is one more degree of freedom present. The lowest energies form two bands with dispersion relations

$$\epsilon_{\pm}(k)=\tfrac{1}{2}E_f+t-t\epsilon_{\mathrm{tb}}(k)$$
$$\pm\{[\tfrac{1}{2}E_f-t+t\epsilon_{\mathrm{tb}}(k)]^2+2V^2\epsilon_{\mathrm{tb}}(k)\}^{1/2}\,. \tag{19}$$

This band structure exhibits the familiar hybridization gap for nonvanishing V. The remaining $D-1$ solutions are degenerate peaks at $\epsilon=2t$. For the special case

$$V^2=2t^2-tE_f\,, \tag{20}$$

the expression Eq. (19) for the two extended bands simplifies. One sign of the square root yields $\epsilon_-(k)=E_f-2t\epsilon_{\mathrm{tb}}$, and the other adds an additional peak at $\epsilon=2t$. Note that relation (20) is *not* identical to Eq. (15), the surface on which the exact solution is obtained. This point will be further discussed below.

Discussion.—The understanding of a true ground state of an interacting system is a very important task. Most of the common approximation schemes are based on a "one-particle language," and it is very instructive to evaluate these in the light of exactly solvable, nontrivial models.

The occupation of the lowest dispersive band [4] with spin σ in the Hubbard model is $\sum_k\langle\psi|c^{\dagger}_{k,\sigma}c_{k,\sigma}|\psi\rangle/\langle\psi|\psi\rangle=N-N_{c,-\sigma}/D$. ($N_{c,\sigma}$ denotes the number of electrons with spin σ.) This result can be hardly understood by one-particle pictures.

Only a few statements about the degeneracy of the eigenstates can be made. The authors assume that for the case $N_c=2N$ (N_c denotes the total particle number) the ground state of the Hubbard model Eq. (11) ($D\geq 3$) is not degenerate; unfortunately, this has not been proven. However, it can be shown that degeneracy is present for $N_c>2N$. When $|\chi\rangle$ is the vacuum, the ground state $|\psi\rangle$ is a spin singlet.

The ground state of the interacting systems is constructed by projection of Slater determinants $|\psi_0\rangle$ [5]. [Note that $\psi^{\dagger}_{R,\sigma}$ is defined by Eq. (6) for the Hubbard case and Eq. (13) for the Anderson model, respectively.]

A Slater determinant is always an eigenstate of a noninteracting Hamiltonian and it is instructive to discuss corresponding noninteracting versions $\mathbf{H}_H^0$ and $\mathbf{H}_A^0(E_f', V')$. It is convenient for that purpose to rewrite the noninteracting Hamiltonians in terms of the "pseudo" Fermi operators $\psi_{R,\sigma}^\dagger$. The simple hopping Hamiltonian then reads

$$\mathbf{H}_H^0 = -2t(2DN - \mathbf{N}_c) + \mathbf{R}_0 , \tag{21}$$

with $\mathbf{R}_0 = 2Dt\sum_{R,\sigma}\psi_{R,\sigma}\psi_{R,\sigma}^\dagger$ being positive semidefinite. By arguments used above it follows that $|\psi_0\rangle$ is the ground state of the noninteracting system [6].

The more complicated Anderson version does not exhibit this property. The analogous representation of the noninteracting Anderson model,

$$\mathbf{H}_A^0(E_f', V') = -2t\left(\frac{2DN}{a^2} - N_e\right) + \frac{1}{a^2}\mathbf{R}_0 , \tag{22}$$

can only be obtained for the parameters $E_f' = 2t - 2Dt\beta^2/a^2$ and $V'^2 = 2Dt^2\beta^2/a^2$, where a and β are taken from the rigorous solution (17). They specify the Slater determinant. Writing the parameter sets E_f, V and E_f', V' as a function of the parameter β/a allows two conclusions: (1) The parameter V' is identical to V, whereas E_f' is "renormalized" to a larger value, $E_f' = \frac{1}{2}E_f + 2t$. As a consequence, the Slater determinant which solves the interacting system (after projection) is the ground state of a *different* noninteracting system. This fact has been seen previously [7]; however, not by rigorous methods. (2) The parameters E_f', V of this system are located on the surface defined by Eq. (20), the relation that simplifies the one-particle spectrum to a single lower band and D δ peaks.

The chemical potential at zero temperature is by definition the energy of an additional particle added to the system. For the Hubbard model, the chemical potential is constant $\mu = 4t$; for the Anderson model it is $\mu = 2t$ if the particle number exceeds $2N$.

This paper discusses two models for highly correlated Fermi systems; however, many more variations including disordered systems may be studied by the method presented here. One additional model of interest is, e.g., the spinless Falicov-Kimball model [8]. Freericks and Falicov [9] proposed that the phase-separated state is the ground state of the one-dimensional case. This proposition has been proven by Brandt [10]; however, it can be shown that for the class of lattices considered here ($D \geq 2$) no phase separation takes place.

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[2] As recent examples, the authors like to mention S. A. Trugman, Phys. Rev. B **42**, 6612 (1990); and E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

[3] The parameter λ allows one to adjust whether the sum $\sum_{R,\sigma} f_{R,\sigma}^\dagger f_{R,\sigma} = (\lambda/E_f)\mathbf{H}_f + (1-\lambda)\mathbf{N}_f$ is interpreted as site-energy term or f-particle number operator.

[4] It is worth mentioning that the operators Eq. (6) may be written as a linear combination of the lowest-band Bloch states *only*.

[5] The operators Eqs. (6) and (13) do not fully obey Fermi commutation rules, nevertheless they are all linear independent, and it is possible to orthogonalize them mutually. Therefore, the states $|\psi_0\rangle$ are in fact Slater determinants.

[6] The state $|\psi\rangle$ may be regarded as the $U = \infty$ version of the Gutzwiller ansatz, which is exact here. Additionally, the exact ratio $\langle\psi|\mathbf{H}_H|\psi\rangle/\langle\psi_0|\mathbf{H}_H^0|\psi_0\rangle = (DN - N_c)/(DN - \frac{1}{2}N_c)$ is identical to the Gutzwiller approximation. For a review on the Gutzwiller method see, e.g., D. Vollhardt, Rev. Mod. Phys. **56**, 99ff (1984).

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