Z. Phys. B 90, 161–166 (1993)

Condensed
Zeitschrift für Physik B Matter

Perovskites in high dimensions

Heavy-fermion vs. $t-J$ fixed point

Roser Valentí, Claudius Gros

Institut für Physik, Universität Dortmund, Postfach 500500, W-4600 Dortmund 50, Federal Republic of Germany

Received: 15 June 1992 / Revised version: 27 July 1992

Abstract. We study the $(D+1)$ band Hubbard model on generalized D-dimensional perovskite structures. We show that in the limit of high dimensions the possible scaling behaviour is uniquely determined via the band-structure and that the model without direct oxygen-oxygen hopping necessarily scales to the cluster limit. A 1/dimension expansion then leads to a $t-J$ like Hamiltonian and the Zhang-Rice analysis becomes rigorous. The large dimension fixed point, in general, still remains the cluster model even when a hopping term between n.n. oxygen-sites is included. Only for a unique ratio of the oxygen onsite energies to the oxygen-oxygen hopping amplitude is a new fixed point possible, corresponding to a heavy-Fermion Hamiltonian.

1. Introduction

The description of the electronic structure of the Cu-O layers of the high-temperature superconductors in terms of simplified model Hamiltonians continues to attract considerable interest. Early on, Anderson [1] discussed the electronic properties of the Cu-oxide superconductors in terms of an effective one-band, Hubbard-like Hamiltonian. This picture has been substantiated on a microscopic basis by Zhang and Rice [2], band structure calculations [3] and experimental NMR and NQR data [4] have been interpreted successfully [4] in terms of an effective one-band model with enhanced antiferromagnetic correlations.

Originally, Zhang and Rice [2] introduced the notion of oxygen holes bound to a central copper-spin (the so-called Zhang-Rice singlet) in order to describe the low lying excitations in terms of a one band $t-J$ Hamiltonian, which they derived by expanding in terms of the copper-oxygen hopping matrix element, t_{dp}. Although this transformation has been confirmed essentially by numerical studies [5], its success has remained puzzling up to now, since formally, the expansion parameter, t_{dp}, is not small in actual calculations.

On the other hand, it has been observed recently [6] that in the limit of large spacial dimensions, D, interesting statements can be made upon the properties of interacting Fermions and that the parameters of the specific model considered need, in general, to be taken as certain scaling functions of the dimension in order to obtain a meaningful and non-trivial model in the limit $D \to \infty$.

Here we consider the possible allowed scalings with dimension, D, of the $(D+1)$-band Hubbard model on generalized D-dimensional perovskite lattices. We find that the scaling behaviour of the hopping amplitudes with dimension is uniquely determined by the band structure [7]. We show rigorously that the Hamiltonian scales to the cluster limit in infinite dimensions for the model with hopping only from copper to n.n. oxygen sites and also for the general model with a direct oxygen-oxygen hopping term included. The expansion around the cluster limit is in a dimensionless hopping amplitude $\sim 1/(2D)$ and the Zhang-Rice picture becomes rigorous.

We find, on the other hand, that for a specific ratio of the oxygen onsite energies to the direct oxygen-oxygen amplitude another fixed point Hamiltonian is possible in the limit of high dimensions, which we identify with a heavy Fermion Hamiltonian.

2. Band structure

We consider a D-dimensional perovskite lattice where the copper sites sit on a D-dimensional hypercubic lattice and the D oxygen sites per unit cell sit in between every two nearest neighbor (n.n.) copper sites. With the n.n. Cu-Cu distance set to unity, the D basis vectors, $\mathbf{T}$, take the form $(1, 0, 0, \ldots)$, $(0, 1, 0, \ldots)$, $\ldots$, $(0, 0, \ldots, 1)$ and the oxygens occupy the sites at $\mathbf{T}/2$.

The $(D+1)$-band Hubbard Hamiltonian on this lattice takes the form

$$H = H_d + H_p + H_{pd}$$

$$H_d = \varepsilon_d \sum_{\mathbf{R},\sigma} d^\dagger_{\mathbf{R},\sigma} d_{\mathbf{R},\sigma} + U_d \sum_{\mathbf{R}} d^\dagger_{\mathbf{R},\uparrow} d_{\mathbf{R},\uparrow} d^\dagger_{\mathbf{R},\downarrow} d_{\mathbf{R},\downarrow}$$

$$H_p = \varepsilon_p \sum_{\mathbf{R},T,\sigma} p^\dagger_{\mathbf{R}+T/2,\sigma} p_{\mathbf{R}+T/2,\sigma}$$

$$H_{dp} = -t_{pd} \sum_{\mathbf{R},\varepsilon,\mathbf{T},\sigma} (d^\dagger_{\mathbf{R},\sigma} p_{\mathbf{R}+\varepsilon\mathbf{T}/2,\sigma} + p^\dagger_{\mathbf{R}+\varepsilon\mathbf{T}/2,\sigma} d_{\mathbf{R},\sigma}). \quad (1)$$

where $\varepsilon = \pm 1$ and the $d^\dagger_{\mathbf{R},\sigma}(p^\dagger_{\mathbf{R}+\varepsilon\mathbf{T}/2,\sigma})$ are creation operators for atomic copper (oxygen) orbitals on site $\mathbf{R}(\mathbf{R}+\varepsilon\mathbf{T}/2)$ with spin $\sigma = \uparrow, \downarrow$. The $\varepsilon_d/\varepsilon_p$ are the onsite energies of the d- and p-level on the copper and oxygen sites respectively, U_d is the onsite-repulsion on the copper sites and $-t_{pd}$ the hopping matrix element between the copper and oxygen sites [8]. We will discuss further below the effect of other matrix elements, like an onsite repulsion on oxygen sites, U_p, a direct n.n. oxygen-oxygen hopping, $-t_{pp}$, and an intersite Coulomb matrix element, V_{dp}.

We are interested in the behaviour of (1) in the limit of large dimensions, $D \to \infty$. For this purpose the matrix elements occurring in (1) are allowed to be functions of the dimension, D. Depending on the scaling (functional dependence) assumed, different fixed points may be obtained in the limit $D \to \infty$. It is reasonable to require [6, 7] that all the terms occurring in the Hamiltonian (1) should yield a nontrivial contribution to the ground-state energy in the limit of infinite dimensions. As an example, in the context of the standard one-band Hubbard Hamiltonian, the onsite-repulsion, U, may be assumed to be independent of dimension, since its contribution is not directly dependent on the coordination number and therefore not strongly dependent on dimension. We will discuss in Sect. 4 that also for the perovskite lattice, where the situation is more subtle, U_d turns out to be scale independent.

The scaling behaviour of the hopping amplitude, $-t_{dp}$ (and in general of all quadratic terms in (1)), is non-trivial and can be determined directly from an analysis of the band-structure [7]. For this, we solve the one-particle eigenvalue problem $H\Psi^\dagger_{\mathbf{k},\alpha,\sigma} = \lambda_\alpha(\mathbf{k})\,\Psi^\dagger_{\mathbf{k},\alpha,\sigma}$ with the Ansatz:

$$\Psi^\dagger_{\mathbf{k},\alpha,\sigma} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} (a_{\mathbf{k},\alpha} d^\dagger_{\mathbf{R},\sigma} + \sum_{\mathbf{T}} e_{\mathbf{k},\mathbf{T},\alpha} p^\dagger_{\mathbf{R}+\mathbf{T}/2,\sigma}), \quad (2)$$

where $\alpha = 1, \ldots, D+1$ denotes the $D+1$ eigenstates per unit cell parametrized by $a_{\mathbf{k},\alpha}$ and $e_{\mathbf{k},\mathbf{T},\alpha}$. The stationary energies, $\lambda_\alpha(\mathbf{k})$, are the solutions of the secular equations

$$(\lambda_\alpha(\mathbf{k}) - \varepsilon_d)\, a_{\mathbf{k},\alpha} = -t_{dp} \sum_{\mathbf{T}'} (1 + e^{-i\mathbf{k}\cdot\mathbf{T}'})\, e_{\mathbf{k},\mathbf{T}',\alpha}$$

$$(\lambda_\alpha(\mathbf{k}) - \varepsilon_p)\, e_{\mathbf{k},\mathbf{T},\alpha} = -t_{dp}(1 + e^{i\mathbf{k}\cdot\mathbf{T}})\, a_{\mathbf{k},\alpha}, \quad (3)$$

which are solved by

$$\lambda_{1,2}(\mathbf{k}) = \frac{\varepsilon_d + \varepsilon_p}{2} \mp \sqrt{(\varepsilon_p - \varepsilon_d)^2/4 + 2t_{dp}^2 \sum_{\mathbf{T}} (1 + \cos(\mathbf{k}\cdot\mathbf{T}))}$$

$$\lambda_{3,\ldots,D+1}(\mathbf{k}) = \varepsilon_p. \quad (4)$$

Note that the interaction, U_d, acts only on the copper sites and that the $D-1$ non-dispersing solutions, $\lambda_{3,\ldots,D+1}$, are superpositions of p-orbitals only. Therefore they have zero spectral weight on the copper sites and factor out of the Hilbert-space. (We will discuss this issue in more detail at the end of this section.) With

$$\gamma(\mathbf{k}) = 1/D \sum_{\mathbf{T}} \cos(\mathbf{k}\cdot\mathbf{T}) \quad (5)$$

we can rewrite the dispersion solutions as

$$\lambda_{1,2}(\mathbf{k}) = \frac{\varepsilon_d + \varepsilon_p}{2} \mp \sqrt{(\varepsilon_p - \varepsilon_d)^2/4 + 2Dt_{dp}^2(1 + \gamma(\mathbf{k}))}. \quad (6)$$

The coefficients for the bonding orbital, $\Psi^\dagger_{\mathbf{k},1,\sigma}$, and anti-bonding orbital, $\Psi^\dagger_{\mathbf{k},2,\sigma}$, are $a_{\mathbf{k},j} = \sqrt{(\lambda_j(\mathbf{k}) - \varepsilon_p)/(2\lambda_j(\mathbf{k}) - (\varepsilon_p + \varepsilon_d))}$ and $e_{\mathbf{k},\mathbf{T},j} = -t\, a_{\mathbf{k},j}\, (1 + e^{i\mathbf{k}\cdot\mathbf{T}})/(\lambda_j(\mathbf{k}) - \varepsilon_p)$, for $j = 1, 2$. It is possible to rewrite the Hamiltonian (1) exactly in terms of the one-particle eigenstates, $\Psi^\dagger_{\mathbf{k},1\ldots D+1,\sigma}$. Note, in fact, that in momentum space the creation operators acting on the copper sites, $d^\dagger_{\mathbf{k},\sigma}$, are a linear superposition of the bonding, $\Psi^\dagger_{\mathbf{k},1,\sigma}$, and antibonding orbitals, $\Psi^\dagger_{\mathbf{k},2,\sigma}$, alone and that we can define generalized oxygen orbitals, $\tilde{p}^\dagger_{\mathbf{k},\sigma}$, orthogonal to the non-bonding orbitals, i.e.

$$d^\dagger_{\mathbf{k},\sigma} = \frac{1}{N} \left(\sqrt{\varepsilon_p - \lambda_1(\mathbf{k})}\, \Psi^\dagger_{\mathbf{k},1,\sigma} + \sqrt{\lambda_2(\mathbf{k}) - \varepsilon_p}\, \Psi^\dagger_{\mathbf{k},2,\sigma} \right)$$

$$\tilde{p}^\dagger_{\mathbf{k},\sigma} = \frac{1}{N} \left(\sqrt{\lambda_2(\mathbf{k}) - \varepsilon_p}\, \Psi^\dagger_{\mathbf{k},1,\sigma} - \sqrt{\varepsilon_p - \lambda_1(\mathbf{k})}\, \Psi^\dagger_{\mathbf{k},2,\sigma} \right), \quad (7)$$

with $N = \sqrt[4]{(\varepsilon_p - \varepsilon_d)^2 + 8Dt_{dp}^2(1 + \gamma(\mathbf{k}))}$ being the appropiate normalization factor. We have then that the Bloch-state $\tilde{p}^\dagger_{\mathbf{k},\sigma}$ is the state orthogonal to the copper-orbital, $d^\dagger_{\mathbf{k},\sigma}$, in the bonding/anti-bonding subspace. We introduce the respective Wannier functions, $\tilde{p}^\dagger_{\mathbf{R},\sigma} = \int d^D k/(2\pi)^D e^{-i\mathbf{k}\cdot\mathbf{R}} \tilde{p}^\dagger_{\mathbf{k},\sigma}$ and $\Psi^\dagger_{\mathbf{R},d,\sigma} = \int d^D k/(2\pi)^D e^{-i\mathbf{k}\cdot\mathbf{R}} \Psi^\dagger_{\mathbf{k},d,\sigma}$ and rewrite the full Hamiltonian in real space as

$$H = H_d + H_{\tilde{p}} + H_{d\tilde{p}} + H_n$$

$$H_d = \varepsilon_d \sum_{\mathbf{R},\sigma} d^\dagger_{\mathbf{R},\sigma} d_{\mathbf{R},\sigma} + U_d \sum_{\mathbf{R}} d^\dagger_{\mathbf{R},\uparrow} d_{\mathbf{R},\uparrow} d^\dagger_{\mathbf{R},\downarrow} d_{\mathbf{R},\downarrow}$$

$$H_{\tilde{p}} = \varepsilon_p \sum_{\mathbf{R},\sigma} \tilde{p}^\dagger_{\mathbf{R},\sigma} \tilde{p}_{\mathbf{R},\sigma}$$

$$H_{d\tilde{p}} = \sum_{\mathbf{R},\mathbf{R}',\sigma} t_{\mathbf{R}-\mathbf{R}'} (d^\dagger_{\mathbf{R},\sigma} \tilde{p}_{\mathbf{R}',\sigma} + \tilde{p}^\dagger_{\mathbf{R},\sigma} d_{\mathbf{R}',\sigma})$$

$$H_n = \varepsilon_p \sum_{\mathbf{R},d=3,\sigma}^{D+1} \Psi^\dagger_{\mathbf{R},d,\sigma} \Psi_{\mathbf{R},d,\sigma} \quad (8)$$

where

$$t_{\mathbf{R}-\mathbf{R}'} = \int \frac{d^D k}{(2\pi)^D} \sqrt{2Dt_{dp}^2(1 + \gamma(\mathbf{k}))}\, e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} \quad (9)$$

is the (long-ranged) hopping amplitude in real space. Clearly, the dynamics of the $(D-1)$ non-bonding orbitals per unit cell described by H_n in (8) does not couple to the bonding and anti-bonding degrees of freedom. The Hamiltonian is block-diagonal and the non-bonding degrees of freedom factor out of the Hilbert space. While this statement is rigorous for the above considered Hamiltonian in all dimensions, a direct oxygen-oxygen hopping amplitude, $-t_{pp}$, would alter this picture, as we

discuss in Appendix B, and the Hamiltonian would become block-diagonal only in the limit of large dimensions, $D \to \infty$. Other Coulomb matrix elements, like U_p or V_{dp}, would also destroy the block-structure of (8) and all the $(D+1)$ degrees of freedom per unit cell would have to be considered at the same time.

3. Cluster expansion

There are several ways of taking advantage of the simplified structure of the Hamiltonian as given by (8).

One possibility is to take the limit $D \to \infty$. We will show in the next section that in this limit the density of states reduces to δ-functions and no propagation occurs, the problem reduces to that of uncoupled clusters with two orbitals (the bonding and the anti-bonding) per cluster (unit cell).

Alternatively, one may show that for $D \to \infty$ the Wannier orbital $\tilde{p}^{\dagger}_{\mathbf{R},\sigma}$ becomes the local superposition, with equal amplitudes, of the $2D$ oxygen orbitals surrounding the central copper-site, $\mathbf{R}$. This is exactly the combination of oxygen orbitals considered by Zhang and Rice [2] in their analysis of the electronic structure of the Cu-oxide superconductors.

Motivated by these findings we now consider Hamiltonian (8) on a perovskite lattice in finite dimension, D, and take $1/(2D)$ as a formal expansion parameter.

Technically, we start from the expression (9) for the hopping amplitudes in real space. We note that $\gamma(\mathbf{k}) \in [-1, 1]$ and that we may therefore expand

$$\sqrt{1+\gamma(\mathbf{k})} = \sum_n \binom{1/2}{n} \gamma^n(\mathbf{k}), \tag{10}$$

where we may write $\gamma(\mathbf{k})$ as $\gamma(\mathbf{k}) = \sum_{\mathbf{T}} (e^{i\mathbf{k}\cdot\mathbf{T}} + e^{-i\mathbf{k}\cdot\mathbf{T}})/2D)$. Substitution of (10) into (9) yields

$$t_{\mathbf{R}-\mathbf{R}'} = \sqrt{2D}\, t_{dp}^2 \left[\delta_{\mathbf{R},\mathbf{R}'} + \frac{1}{2D}\binom{1/2}{1} \delta_{\langle \mathbf{R},\mathbf{R}'\rangle} + \frac{1}{(2D)^2}\binom{1/2}{2} \sum_{\mathbf{R}_1} \delta_{\langle \mathbf{R},\langle \mathbf{R}_1\rangle,\mathbf{R}'\rangle} + \dots \right] \tag{11}$$

Here, the Kronecker $\delta_{\langle \mathbf{R},\mathbf{R}'\rangle}$ is different from zero only for $\mathbf{R}$ and $\mathbf{R}'$ being n.n. sites (on the hypercubic lattice formed by the copper atoms) and the symbol $\langle \mathbf{R}, \langle \mathbf{R}_1\rangle, \mathbf{R}'\rangle$ denotes sets of three lattice sites where both $\mathbf{R}$ and $\mathbf{R}'$ are n.n. of $\mathbf{R}_1$.

We will show in the next section that it is correct to assume the scaling $t_{dp} = \tilde{t}_{dp}/\sqrt{2D}$, with $\tilde{t}_{dp}$ being independent of dimension, D. Then (11) clearly represents an expansion of the real-space hopping amplitudes, $t_{\mathbf{R}-\mathbf{R}'}$, in powers of $1/(2D)$. In lowest order in $1/(2D)$ only hopping between the bonding and the anti-bonding orbital centered on the same site of the hypercubic lattice is present and propagation occurs only at the order $(1/2D)^1$.

In high enough dimensions the formal expansion parameter occurring in (11), $\tilde{t}_{dp}/(2D)$, will inevitably become much smaller than any parameter occurring otherwise in (8), like the charge transfer energy, $\Delta = \varepsilon_d + U_d - \varepsilon_p$, or U_d itself and the Zhang-Rice analysis [2] is then rigorous.

4. Limit $D \to \infty$

Now we proceed to examine the structure of the Hamiltonian, as given by (8), in the limit $D \to \infty$. The correct scaling for U_d is to assume it to be independent of dimension. Note that this is true despite the fact that in the limit of infinite dimensions the single copper-site yields only a vanishingly small contribution, $\sim 1/D$, to the ground-state energy per unit cell. Since the $(D-1)$ non-bonding orbitals factor out of the Hilbert-space, only the two active orbitals per unit cell, the bonding and the anti-bonding orbital, need to be included in the considerations upon scaling.

We are particularly interested in the functional dependence of the hopping amplitude, $-t_{dp}$, on dimension, D. As an illustration of the general procedure, we first review the simpler case of the standard one-band Hubbard-model, where the result is kown [6, 7].

The standard one-band Hubbard model has the dispersion relation $\lambda(\mathbf{k}) = -2tD\gamma(\mathbf{k})$, where $\gamma(\mathbf{k})$ is given by (5). We derive in Appendix A (see also [7, 9]) that in the limit of asymptotically large dimensions the density of states takes the form

$$\rho^{(1)}(\omega) \equiv \int_{-\pi}^{\pi} \frac{d^D k}{(2\pi)^D} \delta(\omega - \varepsilon(\mathbf{k})) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2Dt^2}} e^{-\omega^2/(4Dt^2)}. \tag{12}$$

Clearly, if we assume [6, 7] $\sqrt{2D}t \equiv \tilde{t}$ to be independent of dimension, then the density of states takes the usual gaussian form $\rho^{(1)}(\omega) = e^{-\omega^2/2\tilde{t}^2}/\sqrt{2\pi}\tilde{t}$. To see what happens otherwise we consider $\rho^{(1)}(\omega)$ as a distribution and integrate over a test-function, $g(\omega)$:

$$\int_{-2Dt}^{2Dt} d\omega \rho^{(1)}(\omega) g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\sqrt{2D}}^{\sqrt{2D}} dy e^{-y^2/2} g(\sqrt{2D}t\, y), \tag{13}$$

where we substituted $\omega = \sqrt{2D}t\, y$. Let's assume a general scaling law, $t = \tilde{t}/(2D)^{\alpha}$, and observe from (13) that $\rho^{(1)}(\omega)$ reduces to $\delta(\omega)$ in the limit $D \to \infty$ whenever $\alpha > 1/2$. For $0 < \alpha < 1/2$ (12) and (13) are not well defined in the limit $D \to \infty$ (and not valid for $\alpha < 0$, see Appendix A). It is the critical value $\alpha = 1/2$ which is considered in most studies of the Hubbard-model in infinite dimensions, since then the properties of the model stay non-trivial when the U-term is included.

For the case of the Hubbard model on a D-dimensional perovskite lattice, formulas very similar to (12) and (13) are valid. They can be derived from a general expression which holds for any band-structure, $\lambda(\mathbf{k})$, which depends on the momentum, $\mathbf{k}$, only through $\gamma(\mathbf{k}) \equiv v$ (compare (5) and (6)). Then, as we show in Appendix A,

$$\int_{-\infty}^{\infty} d\omega \rho(\omega) g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\sqrt{2D}}^{\sqrt{2D}} dy e^{-y^2/2} g(\lambda(y/\sqrt{2D})). \quad (14)$$

We recover (13) by substituting in (14) the $\lambda(v) = -2Dtv$ (at $v = y/\sqrt{2D}$) appropiate for the one-band Hubbard model. In infinite dimensions the quantity $\lim_{D\to\infty} \lambda(y/\sqrt{2D})$, needs to be a well defined function of y and uniquely determines the functional form of the density of states. When this quantity is independent of the variable, y, then the density of states reduces to a δ-function in infinite dimensions. For the perovskite lattice we have (see (6)) $\lambda(v) = (\varepsilon_d + \varepsilon_p)/2 \mp \sqrt{(\varepsilon_p - \varepsilon_d)^2/4 + 2Dt_{dp}^2(1+v)}$ and the limiting value

$$\lim_{D\to\infty} \left\{ \frac{\varepsilon_d + \varepsilon_p}{2} \mp \sqrt{(\varepsilon_p - \varepsilon_d)^2/4 + 2Dt_{dp}^2(1 + y/\sqrt{2D})} \right\} \quad (15)$$

needs to be well defined for $D \to \infty$. If we assume that the relative energy scale of the oxygen to the copper onsite energies, $\varepsilon_p - \varepsilon_d$, does not change with dimension (we discuss the alternative case further below) then only for the scaling $t_{dp} = \tilde{t}_{dp}/\sqrt{2D}$ a well defined and non-trivial result is obtained for the density of states in infinite dimensions. Then the density of states becomes

$$\lim_{D\to\infty} \rho(\omega) = \delta\left(\omega - \left(\frac{\varepsilon_p + \varepsilon_d}{2} \mp \sqrt{(\varepsilon_p - \varepsilon_d)^2/4 + \tilde{t}_{dp}^2}\right)\right) \quad (16)$$

for the bonding/anti-bonding band in infinite dimensions. In consequence, the Hubbard Hamiltonian on a infinite-dimensional perovskite lattice reduces to a problem of a hypercubic lattice with two orbitals (bonding/anti-bonding) per unit cell. This problem is a simple version of the Hubbard-star solved recently by Dongen et al. [10]. Note that these clusters are exactly *decoupled* in infinite dimensions and that a spin-spin coupling will occur only when an expansion to finite order in $1/(2D)$ is considered (see Sect. 3).

Now we consider the possibility of scaling the relative onsite energies, $\varepsilon_p - \varepsilon_d$, with dimensions. In this case it is possible [11] to force the system to scale to a standard one-band Hubbard Hamiltonian. To see this, assume that $\varepsilon_d = \sqrt{2D}\tilde{\varepsilon}_d$, $\varepsilon_p = \sqrt{2D}\tilde{\varepsilon}_p$ together with $\tilde{\varepsilon}_p$, $\tilde{\varepsilon}_d < 0$ and $t_{dp} = \tilde{t}_{dp} = \sqrt{|\tilde{\varepsilon}_d \tilde{\varepsilon}_p|}$. Then (15) becomes

$$\lambda_1(y/\sqrt{2D}) \to -\infty$$
$$\lambda_2(y/\sqrt{2D}) \to -t^* y \quad (17)$$

with $t^* = \tilde{t}_{dp}^2/\sqrt{(\tilde{\varepsilon}_p - \tilde{\varepsilon}_d)^2/4 + \tilde{t}_{dp}^2}$. In this scenario the bonding band (and the $(D-1)$ non-bonding bands) have been scaled away to the status of an inert core orbital. Dynamics takes place exclusively in the anti-bonding band with a gaussian density of states, $\rho_2(\omega) = e^{-\omega^2/2(t^*)^2}/\sqrt{2\pi}t^*$. The interaction is the U_d renormalized by the appropriate coherence factors (see (2) and paragraph following (6)). Formally, the scaling to both fixed points, (17) and (16) is allowed. Here in this paper we are specially interested in the consequences of the lattice effects on the fixed point Hamiltonian in infinite dimensions. Since the scaling to (17) scales away all lattice effects we did not consider it in the $1/(2D)$ expansion outlined in Sect. 3.

5. Heavy fermion vs. $t-J$ fixed point

We now include a hopping term between n.n. oxygen sites to the model (1) (see Appendix B for the detailed expression). The band structure is determined by a transcendental equation which cannot be solved analytically in finite dimensions and a block-diagonalization of the Hamiltonian, like (8), is not possible. But in infinite dimension a simplification occurs, as we explain in Appendix B, and an analytic solution is again possible. In this limit the band structure is closely related to that of a model considered by Brandt and Giesekus [12], which may be solved exactly for certain values of the parameters, by the Gutzwiller wavefunction. In the limit of large dimensions the dispersion relation of the bonding/anti-bonding orbitals is (see Appendix B)

$$\lambda_{1,2}(\mathbf{k}) = \frac{\varepsilon_d + \varepsilon_p}{2} - Dt_{pp}(1 + \gamma(\mathbf{k}))$$
$$\mp \sqrt{[(\varepsilon_p - \varepsilon_d)/2 - Dt_{pp}(1+\gamma(\mathbf{k}))]^2 + 2Dt_{dp}^2(1+\gamma(\mathbf{k}))} \quad (18)$$

where $\gamma(\mathbf{k})$ is given by (5). The energies of the $(D-1)$ non-bonding orbitals remain at $\lambda_{3,\ldots,D+1}(\mathbf{k}) \equiv \varepsilon_p$. Here $-t_{pp}$ is the n.n. oxygen-oxygen hopping amplitude.

We discuss first the case of no coupling between the oxygen and the copper sites. Then (18) becomes

$$\lambda_1(\mathbf{k})|_{t_{dp}=0} = \varepsilon_d$$
$$\lambda_2(\mathbf{k})|_{t_{dp}=0} = \varepsilon_p - 2Dt_{pp}(1+\gamma(\mathbf{k})). \quad (19)$$

The anti-bonding solution, $\lambda_2(\mathbf{k})$, depends on the momentum, $\mathbf{k}$, only via $\gamma(\mathbf{k})$ and we can use the same method as in Sect. 4 (see (14)) to determine the possible scalings of t_{pp} and ε_p. From (14) we know that the quantity $\lim_{D\to\infty} \lambda_2(y/\sqrt{2D}) = \lim_{D\to\infty} \{\varepsilon_p - 2Dt_{pp}(1 + y/\sqrt{2D})\}$ must be well defined. Two possibilities arise.

(*i*) No scaling of the zero of energy, ε_p, is considered. Then only $t_{pp} = \tilde{t}_{pp}/(2D)$ is the allowed scaling and $\lim_{D\to\infty} \rho(\omega)|_{t_{dp}=0} = \delta(\omega - (\varepsilon_p - \tilde{t}_{pp}))$.

(*ii*) The zero of energy scales like $\varepsilon_p = 2Dt_{pp}$. Then it is possible to scale $t_{pp} = \tilde{t}_{pp}/\sqrt{2D}$ and the density of states becomes gaussian: $\lim_{D\to\infty} \rho(\omega)|_{t_{dp}=0} = \exp[-\omega^2/(2\tilde{t}_{pp}^2)]/\sqrt{2\pi}\tilde{t}_{pp}$. In this case the onsite energy diverges in the infinite-D limit like $\varepsilon_p = \sqrt{2D}\tilde{t}_{pp}$.

Note that for (*ii*) not only the magnitude, but also the sign of ε_p is related to that of the hopping amplitude, t_{pp}. Such a choice of ε_p effectively cancels the contribution which arises from the hopping within the same unit-cell. Note that in this case the contribution of the non-

bonding orbitals to the ground-state energy, $\sim\varepsilon_p$, diverges too.

Now we consider the case where both t_{dp} and t_{pp} are nonzero. It follows from (14) and (18) that

$$\lambda_{1,2}(y/\sqrt{2D}) = [\varepsilon_p + \varepsilon_d - 2Dt_{pp} - y\sqrt{2D}t_{pp}]/2 \mp \sqrt{[\varepsilon_p - \varepsilon_d - 2Dt_{pp} - y\sqrt{2D}t_{pp}]^2/4 + 2Dt_{dp}^2(1+y/\sqrt{2D})} \tag{20}$$

needs to be well-defined for $D\to\infty$. Again we have two non-trivial choices for the scaling:

(*i*) Consider $\varepsilon_d, \varepsilon_p, \tilde{t}_{pp}, \tilde{t}_{dp}$ general and fixed, $t_{pp} = \tilde{t}_{pp}/(2D)$ and $t_{dp} = \tilde{t}_{dp}/\sqrt{2D}$,

(*ii*) Consider $\varepsilon_d, \tilde{t}_{pp}, \tilde{t}_{dp}$ general and fixed, $\varepsilon_p = \sqrt{2D}\tilde{t}_{pp}$, $t_{pp} = \tilde{t}_{pp}/\sqrt{2D}$ and $t_{dp} = \tilde{t}_{dp}/\sqrt{2D}$.

For (*i*) the infinite-D Hamiltonian consists of independent copper-oxygen clusters on a hypercubic lattice with two orbitals (bonding/antibonding) per unit cell. A 1/dimension expansion would then yield an effective, $t-J$ like Hamiltonian, similar to the case for $t_{pp}=0$ (see Sect. 3).

The density of states for both the bonding and the antibonding band for case (*ii*) is given by the single function

$$\rho(\omega) = \frac{(\omega-\varepsilon_d)^2 + \tilde{t}_{dp}^2}{\sqrt{2\pi}\,\tilde{t}_{pp}(\omega-\varepsilon_d)^2} \exp\left[-\left\{\frac{\omega(\omega-\varepsilon_d)-\tilde{t}_{dp}^2}{\sqrt{2}\,\tilde{t}_{pp}(\omega-\varepsilon_d)}\right\}^2\right] \tag{21}$$

with $\omega\in[-\infty, \varepsilon_d]$ for the (normalized) bonding band, $\int_{-\infty}^{\varepsilon_d} \rho(\omega)\,\mathrm{d}\omega = 1$, and $\omega\in[\varepsilon_d, \infty]$ for the anti-bonding band, $\int_{\varepsilon_d}^{\infty} \rho(\omega)\,\mathrm{d}\omega = 1$. The anti-bonding band, which we may call the conduction electron band, in (21) is centered around $\omega=0$ (note that the zero of energy is fixed) and becomes a pure gaussian in the limit $\tilde{t}_{dp}\to 0$. For $\omega\sim\varepsilon_d$ the density of states is exponentially supressed (and exactly zero at $\omega=\varepsilon_d$) forming a pseudo-gap. For appropiate parameters, like $\varepsilon_d < -\tilde{t}_{pp}$, is the anti-bonding band well separated from the bonding band. The bonding band, we may call it the band of the local level, consists of a sharp peak just below ε_d and goes to $\delta(\omega-\varepsilon_d)$ (see (19)) in the singular limit $\tilde{t}_{dp}\to 0$ (despite the fact that $\rho(\omega)\equiv 0$). Equation (21) describes the density of states for a periodic Anderson model in infinite dimensions. For appropiate values of the parameters involved, in particular the Coulomb-matrix element, U_d, and the density of particles, a state with a large mass-enhancement may be described, corresponding to a mixed valence or a heavy Fermion state.

6. Conclusions

We have considered the $(D+1)$ band Hubbard Hamiltonian on generalized D-dimensional perovskite lattices. In the limit $D\to\infty$ the parametes entering the Hamiltonian need to be scaled as functions of dimension, D, and the functional form of the scaling law is uniquely defined by the one-particle band-structure. We have found that the perovskite structure necessarily scales to the cluster limit for general parameters of the model and that the Zhang-Rice [2] analysis in terms of a $t-J$ type effective Hamiltoninian becomes rigorous as a 1/dimension expansion.

Only for a special point in parameter space, when the onsite oxygen energies, ε_p, and the matrix element for hopping in between n.n. oxygen sites, t_{pp}, fullfil the relation $\varepsilon_p = 2Dt_{pp}$ a scaling to an itinerant fixed-point Hamiltonian is possible. The fixed-point Hamiltonian has then the form of the periodic Anderson model with well separated localized and conduction electron bands. For appropiate densities and onsite Coulomb repulsion, U_d, this Hamiltonian may describe a heavy-Fermion state.

We would like to thank U. Brandt, F. Gebhard, P. Hirschfeld and D. Vollhardt for useful discussions. This work was supported by the Deutsche Forschungsgemeinschaft, by the Minister für Wissenschaft und Forschung des Landes Nordrhein-Westfalen.

Appendix A

Here we calculate the density of states in the limit of infinite dimensions for the one-band Hubbard model and the Hubbard model on a hypercubic perovskite lattice with copper-oxygen hopping, $-t_{dp}$, only.

We observe that in both cases the dispersion relation depends on $\mathbf{k}$ only through $\gamma(\mathbf{k})\equiv\nu\in[-1, 1]$ (compare (5)). For the one-band Hubbard model $\lambda(\mathbf{k}) = -2tD\gamma(\mathbf{k})$ and therefore $\lambda(\nu) = -2tD\nu$. For the anti-bonding orbital of the perovskite lattice (see (6)) $\lambda(\nu) = (\varepsilon_p+\varepsilon_d)/2 + \sqrt{(\varepsilon_p-\varepsilon_d)^2/4 + 2Dt_{dp}^2(1+\nu)}$. The density of states is then

$$\rho(\omega) = \int_{-\pi}^{\pi} \frac{\mathrm{d}^D k}{(2\pi)^D}\,\delta(\omega-\lambda(\mathbf{k})) = \int_{-1}^{1} \mathrm{d}\nu\,\delta(\omega-\lambda(\nu))\,\rho_\gamma(\nu), \tag{22}$$

where $\rho_\gamma(\nu)$ is the density of states for the cosinus band,

$$\rho_\gamma(\nu) = \int_{-\pi}^{\pi} \frac{\mathrm{d}^D k}{(2\pi)^2}\,\delta(\nu-\gamma(\mathbf{k})) = \int_{-\infty}^{\infty} \frac{\mathrm{d}s}{2\pi} \mathrm{e}^{\mathrm{i}s\nu}\left[J_0\left(\frac{s}{D}\right)\right]^D. \tag{23}$$

$J_0(z)$ is the zeroth-order Bessel-function, $J_0(z) \equiv \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}z\cos k}\,\mathrm{d}k/2\pi$, and appears here through the Fourier-representation of the δ-function in (23): $\delta(x) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}sx}\,\mathrm{d}s/(2\pi)$. The factorization in the above equation is a consequence of the simple additative structure of $\gamma(\mathbf{k})$. In the limit $D\to\infty$ we can substitute [7, 9, 13] the expansion $J_0(z) = 1 - z^2/2^2 + z^4/(2^2 4^2) - \ldots = \exp[-z^2/2^2 + z^4\{1/(2^2 4^2) - 1/(2!\,2^4)\} - \ldots]$ in (23). In addition we substitute variables $u=\lambda(\nu)\in[\lambda(-1), \lambda(1)]$ in (22) and use (23) for $\rho_\gamma(\nu)$:

$$\rho(\omega)=\int_{\lambda(-1)}^{\lambda(1)} \mathrm{d}u \frac{\delta(\omega-u)}{|\lambda'(\lambda^{-1}(u))|} \int_{-\infty}^{\infty} \frac{\mathrm{d}s}{2\pi} \mathrm{e}^{\mathrm{i}s\lambda^{-1}(u)} \mathrm{e}^{-s^2/(4D)}. \quad (24)$$

Here $\lambda'(\lambda^{-1}(u))=-2tD$ and $\lambda^{-1}(u)=u/(-2tD)$ for the one-band Hubbard model and

$$\lambda'(\lambda^{-1}(u))=2Dt_{dp}^2/(2u-(\varepsilon_p+\varepsilon_d))$$

and

$$\lambda^{-1}(u)=[((2u-(\varepsilon_p+\varepsilon_d))^2-(\varepsilon_p-\varepsilon_d)^2)/(8Dt_{dp}^2)]-1$$

for the perovskite lattice. In (24) we retained only the lowest order exponent in the reexponentiated small argument expansion of the zeroth order Bessel-function, J_0. This is only allowed when $\lim_{D\to\infty} \lambda(v)/D=0$ for all $v\in[-1, 1]$.

We see from (24) that for all dimensions $\rho(\omega<\lambda(-1))=0$ and $\rho(\omega>\lambda(1))=0$. We can evaluate the u-integral and the s-integral and obtain

$$\rho(\omega)=\frac{1}{|\lambda'(\lambda^{-1}(\omega))|} \int_{-\infty}^{\infty} \frac{\mathrm{d}s}{2\pi} \mathrm{e}^{\mathrm{i}s\lambda^{-1}(\omega)} \mathrm{e}^{-s^2/(4D)}$$

$$=\frac{\sqrt{D/\pi}}{|\lambda'(\lambda^{-1}(\omega))|} \mathrm{e}^{-D(\lambda^{-1}(\omega))^2} \quad (25)$$

for $\omega\in[\lambda(-1), \lambda(1)]$. Substitution of the $\lambda'(\lambda^{-1}(\omega))$ and $\lambda^{-1}(\omega)$ appropiate for the one-band Hubbard model lattice yields (12).

Often it is not so easy to determine directly from (25) the scaling behaviour of the parameters which occur in the expression for $\lambda(v)$. One may then regard $\rho(\omega)$ as a distribution and integrate over a test function, $g(\omega)$. This leads to

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \rho(\omega) g(\omega)=\frac{1}{\sqrt{2\pi}} \int_{-\sqrt{2D}}^{\sqrt{2D}} \mathrm{d}y \mathrm{e}^{-y^2/2} g(\lambda(y/\sqrt{2D})) \quad (26)$$

with the help of the variable substitution, $y^2=2D(\lambda^{-1}(\omega))^2$. This result is generally valid for all band-structures, $\lambda(\mathbf{k})$, which depend on the momentum, $\mathbf{k}$, only via $\gamma(\mathbf{k})$ (see (5)).

Appendix B

Here we solve the Hamiltonian (1) with an additional direct oxygen-oxygen hopping term of the form

$$H_{pp}=-t_{pp} \sum_{\langle \mathbf{R}_p, \mathbf{R}'_p\rangle, \sigma} (p^\dagger_{\mathbf{R}'_p,\sigma} p_{\mathbf{R}_p,\sigma}+p^\dagger_{\mathbf{R}_p,\sigma} p_{\mathbf{R}'_p,\sigma}), \quad (27)$$

the sum is over pairs of nearest neighbor oxygen sites, $\langle \mathbf{R}_p, \mathbf{R}'_p\rangle$, whose positions are given by $\mathbf{R}_p=\mathbf{R}+\varepsilon\mathbf{T}$ and $\mathbf{R}'_p=\mathbf{R}+\varepsilon'\mathbf{T}'$ for a given copper-site, $\mathbf{R}$, any basis vectors $\mathbf{T}$ and $\mathbf{T}'$ of the form $(1, 0, 0, \ldots)$, $(0, 1, 0, \ldots)$, $\ldots$, $(0, 0, \ldots, 1)$ and any $\varepsilon, \varepsilon'=\pm 1$ with the restriction $\varepsilon\mathbf{T}\neq\pm\varepsilon'\mathbf{T}'$.

We solve for the band-structure of (27) together with (1) with the Ansatz given by (2). The stationary energies, $\lambda_\alpha(\mathbf{k})$, are the solutions of the secular equations

$$(\lambda_\alpha(\mathbf{k})-\varepsilon_d)\, a_{\mathbf{k},\alpha}=-t_{dp}\sum_{\mathbf{T}'}(1+\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{T}'})\, \mathrm{e}_{\mathbf{k},\mathbf{T}',\alpha}$$

$$(\lambda_\alpha(\mathbf{k})-\varepsilon_p)\, \mathrm{e}_{\mathbf{k},\mathbf{T},\alpha}=-t_{dp}(1+\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{T}})\, a_{\mathbf{k},\alpha}$$
$$-t_{pp}(1+\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{T}})\sum_{\mathbf{T}'\neq\mathbf{T}}(1+\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{T}'})\, \mathrm{e}_{\mathbf{k},\mathbf{T}',\alpha}. \quad (28)$$

Elimination of the amplitudes, $a_{\mathbf{k},\alpha}$ and $\mathrm{e}_{\mathbf{k},\mathbf{T},\alpha}$ leads to

$$\lambda_\alpha(\mathbf{k})-\varepsilon_d=\sum_{\mathbf{T}}\frac{(2+2\cos(\mathbf{k}\cdot\mathbf{T}))(t_{dp}^2-t_{pp}(\lambda_\alpha(\mathbf{k})-\varepsilon_d))}{\lambda_\alpha(\mathbf{k})-\varepsilon_p-t_{pp}(2+2\cos(\mathbf{k}\cdot\mathbf{T}))}. \quad (29)$$

In general it is not possible to solve (29) analytically and all $(D+1)$ eigenvalues, $\lambda_\alpha(\mathbf{k})$, will be dispersing and no decomposition of the Hilbert-space into non-bonding and bonding/antibonding orbitals occurs. But in the asymptotic limit $D\to\infty$ the denominator of the right-hand side of (29) simplifies due to the relation

$$|\lambda_\alpha(\mathbf{k})-\varepsilon_p|\gg|t_{pp}(2+2\cos(\mathbf{k}\cdot\mathbf{T}))| \quad (30)$$

which holds in infinite-D (see next paragraph). As a consequence, $(D-1)$ non-bonding, non-dispersing eigenvalues $\lambda_{3\ldots D+1}(\mathbf{k})\equiv\varepsilon_p$ solve (28) for $D\to\infty$ and the bonding/anti-bonding bands are given by (18). The Hamiltonian (1) together with (27) becomes block-diagonal and a representation similar to (8) can be found.

Equation (30) is consistent in particular with both the possible scalings discussed in the text, namely

(*i*) $\lambda_\alpha(\mathbf{k})$, $\varepsilon_p\sim(2D)^0$ and $t_{pp}\sim(2D)^{-1}$.
(*ii*) $\lambda_\alpha(\mathbf{k})$, $\varepsilon_p\sim(2D)^{1/2}$ and $t_{pp}\sim(2D)^{-1/2}$.

The simplification (30) occurring in high dimensions can be understood easily. The term $-t_{pp}(2+2\cos(\mathbf{k}\cdot\mathbf{T}))$ in the denominator of the right hand side of (29) is a direct consequence of the restriction $\varepsilon\mathbf{T}\neq\pm\varepsilon'\mathbf{T}'$ of the matrix elements in (27) which leads to the restriction $\mathbf{T}'\neq\mathbf{T}$ in the last sum in (28). But this restriction is of order $1/D$ and may be neglected in high dimensions.

References

1. Anderson, P.W.: Science **235**, 1196 (1987)
2. Zhang, F.C., Rice, T.M.: Phys. Rev. B **37**, 3759 (1988)
3. For a review see Pickett, W.: Rev. Mod. Phys. **61**, 433 (1989)
4. See Millis, A.J., Monien, H.: Phys. Rev. B **45**, 3059 (1992) for references and discussion
5. See e.g. Bacci, S.B., Gagliano, E.R., Martin, R.M., Annett, J.F.: Phys. Rev. B **44**, 7504 (1991) and references therein
6. Metzner, W., Vollhardt, D.: Phys. Rev. Lett. **62**, 324 (1989)
7. Müller-Hartmann, E.: Z. Phys. B – Condensed Matter **74**, 507 (1989)
8. Any change of the sign of $-t_{pd}$ with direction due to the symmetry of the d-level or p-level orbitals are thought to be gauge-transformed away
9. Wolff, U.: Nucl. Phys. B **225**, 391 (1983)
10. Van Dongen, P.G.J., Vergés, J.A., Vollhardt, D.: Z. Phys. B – Condensed Matter **84**, 383 (1991)
11. Gebhard, F.: Private communication
12. Brandt, U., Giesekus, A.: Phys. Rev. Lett. **68**, 2648 (1992)
13. Brandt, U., Hülsenbeck, G.: Private communication