3 Model Hamiltonians and Basic Techniques

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1   Motivation

The problem of interacting electrons in realistic systems is a difficult one. Although conventional Bloch band theory with its roots dating back to the 1920s (see Ref. [1] for a historical review) is very successful in describing many so-called weakly correlated materials, the intricate phenomenology of electronic systems that display signatures of strong correlations are basically outside that scope. First-principles or *ab-initio* approaches to tackle such systems on a smiliar level of sophistication as their weakly correlated neighbors is highly non-trivial and the central topic of this school. In this context, model Hamiltonians play an essential role by, loosely speaking, bridging the gap between the possible to the (nearly) impossible. Their justification can in principle be categorized more concretely by

(i) the tremendous complexity of materials systems on a microscopic level because of the large numbers of various degrees of freedom in often low-symmetry environments that asks for simplifications to discuss the dominant physics of interest.

(ii) the condensation of different robust physical mechanisms in simplified mathematical terms in order to look for new physical processes via their facinating mutual interplay.

Both theoretical perspectives allow for a predictive character in the use of models, yet the first one is somewhat more directly associated with given materials problems. Therefore we want to concentrate thereon, namely on model Hamiltonians geared to simulate the key physics of notoriously complicated complete Hamiltonians of large-scale interacting systems. Note that a model approach not always has to cover only low-energy scales, but that often also high-energy excitations are of vital interest. In addition, here we are aiming at the full quantum nature of the problem and leave possible classical approximations (e.g., Ising model in zero field [2], etc.), though often also interesting, aside.

Lets indeed start from the complete Hamiltonian $\mathcal{H}$ of a condensed matter system with N_e electrons and N_K nuclei on a lattice with position vectors $\mathbf{R}_\alpha$. In first quantization the problem reads

$$\mathcal{H} = \underbrace{-\sum_{\alpha}^{N_K} \frac{\hbar^2 \Delta_\alpha}{2M_\alpha} + \frac{1}{2}\sum_{\substack{\alpha\alpha' \\ \alpha\neq\alpha'}} \frac{Z_\alpha Z_{\alpha'} e^2}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}}_{=:\mathcal{T}_K + \mathcal{V}_{KK} =: \mathcal{H}_K} \underbrace{-\sum_{\alpha\mu} \frac{Z_\alpha e^2}{|\mathbf{R}_\alpha - \mathbf{r}_\mu|}}_{=:\mathcal{V}_{Ke}} \underbrace{-\sum_{\mu}^{N_e} \frac{\hbar^2 \Delta_\mu}{2m} + \frac{1}{2}\sum_{\substack{\mu\mu' \\ \mu\neq\mu'}} \frac{e^2}{|\mathbf{r}_\mu - \mathbf{r}_{\mu'}|}}_{=:\mathcal{T}_e + \mathcal{V}_{ee} =: \mathcal{H}_e} \quad ,$$

$$\tag{1}$$

composed of a pure part $\mathcal{H}_K$ for the nuclei, a pure electronic part $\mathcal{H}_e$ as well as the coupling $\mathcal{V}_{Ke}$ thereof. The Born-Oppenheimer approximation (BOA) [3] allows a decoupling of the problem for the nuclei from the electrons, ending up with an electronic Hamiltonian of the form

$$H_e = H_e(\{\mathbf{R}\}) := \mathcal{H}_e + \mathcal{V}_{Ke} \quad , \tag{2}$$

where the set $\{\mathbf{R}\}$ of lattice points is a mere fixed parameter set for the given electronic problem. The periodic lattice potential $\mathcal{V}_{Ke}$ is then often denoted as *external potential* v_{ext}, to highlight

the electronic-system character. The remaining lattice part of $\mathcal{H}$ eventually leads to phonon excitations and their interactions, which we will not cover in this overview. Only in section 3.3 a brief discussion of modelized electron-phonon coupling, i.e., physics beyond the BOA, will mildy touch this matter.

The sobering news is that after the decoupling from the lattice degrees of freedom the solid-state problem of interacting electrons within an external potential is still much too complicated. In band theory it is assumed that H_e may be written as a sum of effective single-particle terms, i.e., the electron-electron interaction $\mathcal{V}_\mathrm{ee}$ as a two-particle operator is transformed into a one-particle form. Although for ground-state properties such an exact transformation *in principle* exists (see the chapter on density functional theory), so far, however, any practical approximation leads to severe failures for correlated solid-state systems. Not only is the exact analytical treatment of the true H_e impossible, also tough numerical methods surrender to the explosion of the associated Hilbert space in this technically very demanding potential landscape of a realistic solid. Unlike in quantum chemistry, where these numerical techniques for atoms and smaller molecules are often still feasible (however nowadays also with a huge amount of labor, see e.g. [4] for an introduction), condensed matter theory is in need of model approaches.

Thus in the following sections we will deal with ways of simplifying H_e in order to squeeze some interesting physics out of it. While sections 2 and 3 cope with the definition of the Hubbard model and its friends, sections 4 and 5 deal with first simple and not so simple tools for the actual solutions. In fact, albeit we just emphasized the complexity of realistic systems, solving, once derived, model Hamiltonians is very far from being easy and a whole community in theoretical condensed matter physics is devoted to this. In the end it is mainly about changing an almost utopian problem into a less utopian one.

2 Introduction to the single-band Hubbard model

Since there is a whole zoo of model Hamiltonians available, we have to limit the discussion to a certain subset. As our main interest in this school is in problems where the interplay between kinetic energy gain and cost of Coulomb interaction is central, it is meaningful to circle the discussion around the Hubbard model. Excellent accounts of pure spin models can be found elsewhere (see e.g. the books [5–7]).

2.1 Competition between itinerancy and localization

Before presenting a heuristic derivation of the basic Hubbard model its useful to provide an intuitive view on the main driving forces that govern interacting electron systems in a solid.
When placing atoms in regular periodic arrays, the first obvious deviation to atomic physics is due to symmetry, namely the splitting of states because of the emerging crystal field . The latter competes usually with the exchange splittings responsible for Hund's rules as well as with the spin-orbit interaction. In the following we assume the general understanding that for *spd* systems intermediate crystal-field strengths apply. Thus Hund's first and second rule are vital

and the still smaller crystal field dominates over the spin-orbit interaction.

Because of the Heisenberg uncertainty principle the electrons are in favor of minimizing their kinetic energy through dislocation, i.e., hopping processes between different atoms are preferable, leading eventually to crystal bonding. However as in atomic physics, whenever electrons come close the Coulomb energy raises due to the mutual interaction. Hence the overall movements within the electronic system are quite intricate and usually highly correlated. But there are two limits when everything becomes much simpler. If the effective Coulomb interaction in the system is very well screened, in a simple picture one may assume that the electrons are rather free to optimize their kinetic energy irrespective of the restrictions imposed by interaction. Note that one truly has to invoke the quasiparticle concept of Landau Fermi-liquid theory (see e.g. [8]) to fully justify such a view, since the screening is itself mediated by the electronic system. An even simpler limit is provided by the absence of sufficient screening processes in a commensurable filling scenario. The latter means an integer ratio between the number of electrons N_e and the number of lattice sites N_l. Then the electrons' tendency to leave their lattice site and hop around the lattice is approaching zero and an insulating state of matter results. This electron localization in real space, termed *Mott insulator*, is quite different from the commonly known band-insulating state. In a band insulator the absence of electrical conductivity is based on the complete filling of a band of effective single-particle Bloch states and the existence of an HOMO-LUMO gap. A Mott insulator is a quite different beast with a charge gap that is not governed by (renormalized) hybridization effects but which originates from the (renormalized) Coulomb interaction between the electrons.

In summary, we expect the competition between the itinerant and the localized character of the electrons as the vital ingredients to get a hold on the key physics of many correlated electron systems. In the following the concentration will be therefore on the simplified coherent modeling of this rivalry in mathematical terms, leaving other more specific mechanisms aside. The very basic model Hamiltonian that is tailored to serve this goal is the so-called single-band Hubbard Hamiltonian.

2.2 Heuristic derivation

Instead of approximating H_e of eq. (2) as a sum of single-particle terms, another viewpoint is taken now. The aim is to keep the explicit many-particle structure of the full Hamiltonian, but to chop off those terms that are not vital for the basic modeling we outlined in the last subsection. Since best suited for many-body systems, we therefore start by writing H_e in second quantization[1] as

$$H_e = - \sum_{\alpha\beta ab\sigma} t^{L_a L_b}_{\mathbf{R}_\alpha \mathbf{R}_\beta} c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c_{\mathbf{R}_\beta L_b \sigma} + \frac{1}{2} \sum_{\substack{\alpha\beta\gamma\delta \\ abcd\sigma\sigma'}} V_{ee}(\{\mathbf{R}, L\}) \, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c^\dagger_{\mathbf{R}_\beta L_b \sigma'} c_{\mathbf{R}_\delta L_d \sigma'} c_{\mathbf{R}_\gamma L_c \sigma} \; . \quad (3)$$

Here the electron creation and annihilation operator $c^{(\dagger)}$ is represented in a localized Wannier basis $\varphi(\mathbf{r})$ in real space, marked by lattice site $\mathbf{R}$, orbital character L and spin projection σ.

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[1]In the following hermiticity of the hopping term is assumed to be enforced.

While the first sum over single-particle terms carries the kinetic energy as well as the interaction with the periodic lattice potential, the second sum describes the electron-electron Coulomb interaction. Note that we do not allow for spin-dependent hopping processes, as here magnetic effects should emerge from the interacting part. The respective matrix elements read

$$
t_{\mathbf{R}_\alpha \mathbf{R}_\beta}^{L_a L_b} = \int d\mathbf{r}\, \varphi_{\mathbf{R}_\alpha L_a}^*(\mathbf{r}) \left\{ \frac{\hbar^2 \Delta}{2m} - v_{\text{ext}}(\mathbf{r}) \right\} \varphi_{\mathbf{R}_\beta L_b}(\mathbf{r}) \quad , \tag{4}
$$

$$
V_{ee}(\{\mathbf{R}, L\}) = \int d\mathbf{r} d\mathbf{r}'\, \varphi_{\mathbf{R}_\alpha L_a \sigma}^*(\mathbf{r})\, \varphi_{\mathbf{R}_\beta L_b \sigma'}^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \varphi_{\mathbf{R}_\gamma L_c \sigma'}(\mathbf{r}')\, \varphi_{\mathbf{R}_\delta L_d \sigma}(\mathbf{r}) \quad . \tag{5}
$$

Everybody with a basic training in quantum mechanics immediately realizes that its impossible to work out the solution for such a problem with so many degrees of freedom. Whereas the single-particle term is feasible, resulting in a simple form of band theory, the two-particle part is the tough one. From a formal theoretical point of view, one proper method for simplification would be to integrate out high energy degrees of freedom within the spirit of the renormalization-group theory. However for general materials systems this proves unmanageable. Moreover, since we want to study metallic and gapped systems on an equal footing such a recipe is inadequate at the present level. The natural way of dealing with it is by applying two key observations:

(1) In order to get a very first understanding of competing itinerancy and localization, a full multi-orbital structure is not necessary. Furthermore, one can limit the discussion to only nearest-neighbor (NN) hopping of the electrons.

(2) The Coulomb interaction between two electrons is usually strongest if both come close in the same localized Wannier orbital. With distance the interaction rapidly decays for many systems also due to efficient screening processes of other interfering electrons.

We therefore take a rather radical approach and assume a model system with NN hoppings between only one Wannier orbital per identical sites, e.g. a model lattice of hydrogen atoms, and keeping solely the on-site Coulomb matrix element $V_{\text{ee}}(\mathbf{R}, \mathbf{R}, \mathbf{R}, \mathbf{R}){=}{:}U$. In what follows, to keep notations simple it is customary to label lattice sites with $(i,j,\dots)$ and introduce the particle-number operator $n{=}c^\dagger c$. With the given dramatic simplifications the complicated Hamiltonian (3) may then be cast into

$$
H_{\text{hub}} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \varepsilon_0 \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad . \tag{6}
$$

This is the famous single-band Hubbard model, named after J. Hubbard due to its seminal work[2] [9]. It has only two explicit relevant parameters, namely the hopping amplitude t and the on-site Coulomb interaction, the so-called Hubbard U. Note that the second term scaling by the local single-particle level energy ε_0 (stemming from $t_{\mathbf{R}_\alpha \mathbf{R}_\alpha}$ in eq. (3)) is not strictly mandatory.

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[2]Note however that many authors independently came up with very similar Hamiltonians at around the same time, including P. W. Anderson, M. C. Gutzwiller and J. Kanamori.

Because it only amounts to a shift in energy, one could easily choose $\varepsilon_0{=}0$ without changing the model properties. The braces in the first sum denote it only runs over NN sites.

Its innocent appearance compared to the full form (3) should not mask the fact that solving the Hubbard model is a very tough job. There is only an exact analytical solution in one dimension (1D) and a numerical exact approach for the infinite-dimensional case which is just the dynamical mean-field theory (DMFT) this school is to a large part devoted to. Sadly enough, the two- and three-dimensional cases, closest to many strong correlation problems in nature, are the really hard nuts to crack. The difficulty arises from the difference of the summation parts. While the first and second sum may easily be diagonalized in *reciprocal space*, the same easy diagonalization can be performed for the third sum, however, on every lattice site in *real space*. In other words, the first sums pose a standard band-theory problem, whereas the third sum may be interpreted as a standard quantum-chemical one. Diagonalizing both parts simultaneously in 2D and 3D appears to be impossible.

Besides t and U there are other implicit "parameters" for the model, such as the lattice type (e.g., square, triangular, fcc, etc.) and the filling $n{=}N_e/N_l$ (not to be confused with the particle-number operator). A very important setup in this respect is the so-called half-filled case, where $n{=}1$, i.e., there is one electron per lattice site (and hence per orbital). In that integer filling regime the system is in principle susceptible to a Mott-insulating state, whereas the rather trivial integer fillings $n{=}0,2$ denote band insulators. Its important to realize that at any other filling no insulating state is reachable for finite t in this model. Since then there will be always double occupations of lattice sites coexisting with single occupations and thus the possibility to lower the total energy via hopping processes.

There is a huge literature on the Hubbard model which in this small review we do not dare to approach. Very detailed overviews can e.g. be found in the books of Fazekas [6] and Gebhard [10].

2.3   Some model limits and basic excitations

When trying to understand a given model it is always a good idea to first examine the limiting regimes. Restricting the discussion to the interesting half-filled $n{=}1$ case, it is obvious that the ratio U/t serves as a perfect marker. For a certain lattice type one would rather use the bandwidth $W{\sim}t$ in the denominator, yet we try to keep things simple and do not choose a specific lattice. In order to render the discussion a bit more quantitative, let us focus on computing the zero-temperature *spectral function* $A_\sigma(\mathbf{k}, \omega)$ given by the following expression[3,4]

$$A_\sigma(\mathbf{k}, \omega) = \begin{cases} A_\sigma^+(\mathbf{k}, \omega) = \sum_m |\langle \Psi_m^{(N_e+1)}|c_{\mathbf{k}\sigma}^\dagger|\Psi_0\rangle|^2\, \delta(\omega - \omega_{m0}) & \text{for } \omega \geq 0 \\[2mm] A_\sigma^-(\mathbf{k}, \omega) = \sum_m |\langle \Psi_m^{(N_e-1)}|c_{\mathbf{k}\sigma}|\Psi_0\rangle|^2\, \delta(\omega - \omega_{0m}) & \text{for } \omega < 0 \end{cases}, \quad (7)$$

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[3]This form is exact in the thermodynamic limit, where the energy differences upon particle addition and removal are identical (see e.g. [11]).

[4]The convention $\hbar{=}1$ is used.
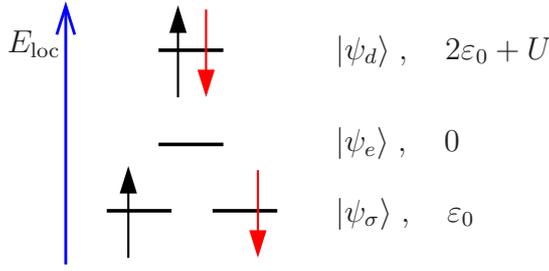
Fig. 1: *Level diagram for a single lattice site with one orbital.*

with $c_{\mathbf{k}\sigma}^{(\dagger)}$ now creating/annihilating electrons with wave vector $\mathbf{k}$ and spin projection σ. This function provides information about the system's energy distribution via summation over processes after adding and removing an electron to the ground-state wave function $|\Psi_0\rangle$. Thereby the $|\Psi_m\rangle$ denote excited $(N_e \pm 1)$-particle eigenstates with eigenenergies ω_{m0}, ω_{0m} with respect to the ground state. Of course, these states are unbelievably complicated for generic U/t, however everything becomes rather simple for two limiting cases:

Fermi-gas limit U=0. The problem reduces to the simplest band-theoretical form since the Hubbard model looses its interaction term. Hence $\mathbf{k}$ is a good quantum number and creating/annihilating electrons according to (7) already produces eigenstates of the system, the well-known Bloch states. Since $\langle\Psi_{(m0)}|c_{\mathbf{k}\sigma}^{(\dagger)}|\Psi_{(m0)}\rangle$ equals one for the associated eigenstate and zero otherwise, the k-integrated spectral function $\rho_\sigma(\omega)$ reduces to[5]

$$\rho_\sigma(\omega) = \sum_{\mathbf{k}} A_\sigma(\mathbf{k}, \omega) = \sum_{\mathbf{k}} \delta(\omega - \varepsilon_{\mathbf{k}}) \quad , \tag{8}$$

which is the familiar electronic density of states (DOS) from single-particle theory for the band dispersion $\varepsilon_{\mathbf{k}}$. So one recovers the good old band-theoretical result for a metallic state based on a simple NN hopping. Because interactions among the electrons are completely absent, one usually refers to this solution also as the Fermi gas. This means that in real space the local site occupations, i.e., empty, single and double, are according to the statistics of a non-interacting lattice gas.

Atomic limit t=0. This is just the opposite case, no hopping allowed and therefore insulating by default. But now we are facing a truly interacting problem. Albeit a purely local one since obviously the whole job is easily separable into a sum of N_l isolated atomic problems. There are four states per site, which are summarized with their energetics in Fig. 1. For the computation of $\rho_\sigma(\omega)$ one first needs to apply the Fourier-transformation rule $\sqrt{N_l}\, c_{\mathbf{k}\sigma}^{\dagger} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{R}\sigma}^{\dagger}$ (and c.c. for $c_{\mathbf{k}\sigma}$) to eq. (7) and the problem can be examined for the two brances $\omega \lessgtr 0$ as

$$\rho_\sigma(\omega) = \begin{cases} \sum_{\mathbf{R}}\langle n_{\mathbf{R}\bar\sigma}\rangle|\langle\psi_d|c_{\mathbf{R}\sigma}^{\dagger}|\psi_{\bar\sigma}\rangle|^2\,\delta(\omega - \omega_{d\bar\sigma}) = \sum_{\mathbf{R}}\langle n_{\mathbf{R}\bar\sigma}\rangle\,\delta(\omega - (\varepsilon_0 + U)) \\[2ex] \sum_{\mathbf{R}}\langle n_{\mathbf{R}\sigma}\rangle|\langle\psi_e|c_{\mathbf{R}\sigma}|\psi_\sigma\rangle|^2\,\delta(\omega - \omega_{e\sigma}) = \sum_{\mathbf{R}}\langle n_{\mathbf{R}\sigma}\rangle\,\delta(\omega - \varepsilon_0) \end{cases} , \tag{9}$$

since for n=1 the degenerate $|\psi_{\sigma,\sigma'}\rangle$ forms the local ground state. Thus there are only δ-Peak excitations at ε_0 and $\varepsilon_0 + U$ as expected for an atomic problem. Contrary to the Fermi-gas limit

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[5]Throughout the text the proper normalization of $\mathbf{k}$- and $\mathbf{R}$-sums to the number of k/R-points is assumed.
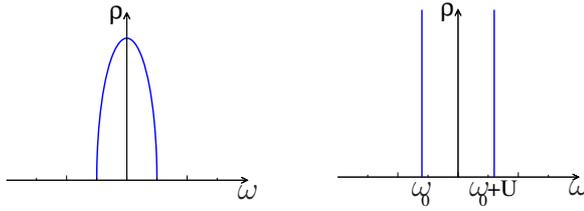
Fig. 2: *Schematic local spectral function for the Fermi-gas limit $U=0$ (left) and the atomic limit $t=0$ (right) of the Hubbard model at half filling.*

now only single occupied sites appear in the real space ($n=1$)-ground state, because double occupations cost energy.

The local spectral function $\rho_\sigma(\omega)$ for the two limits is depicted in Fig. 2. Note again the very different nature of excitations: whereas for $U=0$ there are ordinary Bloch excitations in k-space forming a rather broad band, for $t=0$ the system shows local multiplet excitations in r-space. Now what happens away from these limits ? A simplistic first guess would be to more or less overlay the limiting spectra to mediate between them, whereby one has to take into account that any finite t will broaden spectral peaks in energy. The pictures that emerge presumably look like the ones shown in Fig. 3. Turning on U when starting in the Fermi gas has two main effects. First it leads to *band narrowing* (or the Brinkman-Rice effect [12]), because hopping processes are now somewhat supressed due to the cost of energy when there are necessarily double occupations formed which are penalized by U. Secondly, multiplet excitations gradually emerge at higher energies already in the metal, since spectral weight that is now missing in the band-like excitations is transfered into the former. This spectral-weight transfer is a hallmark signature of strongly correlated electron systems.

One refers to the renormalized band part at low energy, i.e., close to the Fermi level ε_F, as *quasiparticle excitations* and to the smeared multiplet excitations at higher energies to *Hubbard excitations* or *Hubbard bands*. At very large U/t the system finally undergoes a Mott-insulating transition (MIT). The quasiparticles that remain close to ε_F until the Mott insulator sets in still may be marked with wave vector **k**, but now have finite lifetime due to the fact that $c_{\mathbf{k}\sigma}^{(\dagger)}$ do not anymore create/annihilate eigenstates of the solid. In other words, Bloch's theorem does not hold on the interacting lattice. The broader Hubbard bands are doomed with even shorter lifetime, since the incoherent multiplets do not propagate well on the lattice.

The limit $U/t \gg 1$ deserves indeed further discussion. It is important to realize that this case is of course very different from the atomic limit of decoupled lattice sites. Therefore the Mott-insulating state at half filling is still an unique state of condensed matter. In order to approach this very strongly correlated limit for arbitrary filling theoretically, a systematic perturbative
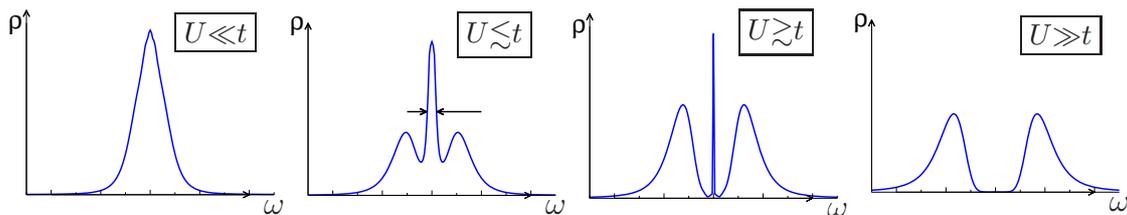
Fig. 3: *Local spectral function for the Hubbard model on a Bethe lattice with increasing U at half filling $n=1$. The graphs were obtained within DMFT.*

expansion of the Hubbard model in t/U may be performed (for details see [5, 6, 10]). For convenience setting ε_0=0, this leads to the *t-J model*

$$H_{\text{tj}} = P \left[-t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} - \frac{t^2}{U} \sum_{\langle ijk \rangle} \left(c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} \right) \left(c_{j\downarrow} c_{k\uparrow} - c_{j\uparrow} c_{k\downarrow} \right) \right] P \quad . \tag{10}$$

The projection operator P restricts the whole configuration space to only those configurations with empty and single occupied sites. Some theorists believe that this model is a good starting point to enter the physics of cupper-oxide high-temperature superconductors [13]. In the Mott insulator at half filling only spin excitations appear at low-energy and this model further reduces to the *antiferromagnetic quantum Heisenberg model*[6]

$$H_{\text{heis}} = \frac{2t^2}{U} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S_j} \quad , \tag{11}$$

with the spin operators defined as $S^\mu_i = 1/2 \sum_{\sigma\sigma'} c^\dagger_{i\sigma} \tau^\mu_{\sigma\sigma'} c_{i\sigma'}$, where $\tau^\mu_{\sigma\sigma'}$ are the elements of the ($\mu = x, y, z$) Pauli matrices. The coupling constant is also most often written via the superexchange parameter $J = 4t^2/U > 0$. So in the end the well-known Heisenberg model is contained in the minimal Hubbard model. For a deeper discussion of the *t-J* and the Heisenberg model we again refer to [4–6, 10]) and references therein.

3   Relatives and extensions of the Hubbard model

In the following sections we briefly want to discuss further Hamiltonians related to the Hubbard model and also extensions of the latter. This is important because many materials problems obviously just do not easily boil down to a simple Hubbard-model form. For instance already the assumption of only NN hopping is rather restrictive and many system display more sophisticated hopping paths. However it is easy to lift this restriction by taking more distant hoppings (e.g., obtained from a Slater-Koster parametrization [14]) into account and writing

$$H_{\text{hub}} = -\sum_{ij,\sigma} t_{ij} \, c^\dagger_{i\sigma} c_{j\sigma} + \varepsilon_0 \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad . \tag{12}$$

The allowance of more than one orbital per site needs some more thinking and will be discussed in section 3.2. But before we want to have a look on a natural companion of the Hubbard Hamiltonian that has also relevance for the DMFT construction.

3.1   Anderson Hamiltonian

Instead of considering an ensemble of fully correlated lattice sites, it is also very instructive to investigate so-called *impurity models.* There only a few down to one correlated lattice site(s) exist within a given host lattice that supports otherwise rather weakly correlated sites. Since we

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[6]Constant energy shifts are neglected.

are here mainly interested in the competition between localization and itinerancy, it is assumed that the electrons stemming from the weakly correlated sites form a simple metallic state. Motivated by experiments on the local-moment behavior of correlated impurity atoms in metals (such as e.g. Fe atoms in copper) and after preliminary theoretical work, P. W. Anderson set up an interacting model Hamiltonian for the single-impurity problem [15], which reads

$$H_{\text{and}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \varepsilon_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\mathbf{k}\sigma} \left(V_{\mathbf{k}d}\, c_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} + V_{\mathbf{k}d}^{*}\, d_{\sigma}^{\dagger} c_{\mathbf{k}\sigma} \right) \quad . \tag{13}$$

This Anderson Hamiltonian has in principle similar components as the Hubbard Hamiltonian, but note that there is now only one correlated impurity site with atomic level ε_d and Hubbard interaction U, embedded in a Fermi sea of band electrons with dispersion $\varepsilon_{\mathbf{k}}$. The important ingredient is now of course the coupling or hybridization between these two parts, marked by the matrix element $V_{\mathbf{k}d}$. This model is usually suited to describe isolated rather well-localized d- or f-levels within a metallic host. A more stringent introduction is e.g. provided in reference [16], here we only try to sketch the main features of the Hamiltonian.

The atomic states of the isolated impurity are the same as the ones depicted in Fig. 1. Let us assume again a local filling $n{=}1$ of the impurity ion. Upon hybridization with the conduction sea, the impurity level broadens by Δ. When turning on U one again faces a competing situation: for large U/Δ the single broadened level will split into two with energy separation U, giving rise to a mean-field local moment $m{=}n_{d\uparrow}{-}n_{d\downarrow}$. The critical value U_c for this to happen can be calculated in mean field as $U_c{=}\pi\Delta$. Hence the appearance of local moments for impurity atoms in a host metal depends on the strength of the screened on-site impurity Coulomb interaction as well as on the impurity-host hybridization. The latter may often be drawn already from the DOS of the host system.

Beyond mean field, the Anderson Hamiltonian paves the road towards even deeper physics. Namely, the splitting of the impurity level is such that a resoncance at the Fermi level remains due to adiabaticity, in resemblance to what we have seen in the Hubbard model on the lattice in Fig. 3. What we identified there as the quasiparticle excitation on the lattice is now called the *Kondo resonance* and is a bit harder to grasp. The intuitive idea behind it is that when the local moment forms at large U, at some point local charge fluctuations become only virtual and the excitations that remain due to the impurity-host coupling are solely of spin nature. In that sense the Kondo resonance is based on a highly correlated quantum-fluctuating many-body state. In fact it can be shown that there is a well-defined theoretical formalism, the so-called Schrieffer-Wolff transformation (see e.g. [16] for details), that allows to reduce the Anderson Hamiltonian at very large U/Δ to the following spin-interacting form[7]

$$H_{\text{kondo}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + J\, \mathbf{s}_{\text{host}} \cdot \mathbf{S}_d \quad , \tag{14}$$

where $\mathbf{s}_{\text{host}}$ denotes the spin density due to the conduction electrons at the impurity site. This is the Kondo Hamiltonian named after J. Kondo due to its famous analysis of the relation be-

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[7]The formal k dependence of J is here neglected.

tween local-moment scattering and the resistivity minimum in such metallic impurity-host systems [17]. Note that the spin interaction is antiferromagnetic, i.e., $J>0$. Unfortunately there is no space in the present scope to discuss the fascinating physics of the Kondo effect in more detail and so we just refer to Coleman's discussion [16] or even more extended surveys like e.g. the book by Hewson [18].

3.2 Multi-band Hubbard Hamiltonians

Let us now come back to the problem of correlated sites building up a periodic lattice (in fact, there are also Kondo lattices, but thats a bit a different story (see, e.g., [6])). There are only a few cases of materials-specific problems where focussing the theoretical discussion on sole single-band properties is then truly sufficient. For instance, many correlated materials studies deal with the $3d$-shell of transition-metal ions in a certain crystal-field evironment. There, as already noted, one expects the splitting of the levels according to symmetry (see Fig. 4). Though it is often legitimate then not to invoke the full five-orbital shell as correlated subspace, but to focus on the three-orbital t_{2g} or the two-orbital e_g manifold. But reducing it to only one effective orbital/band is often too much asked. Although the single band Hubbard model is very important in condensed matter physics, in most cases the hybridizations among orbitals in realistic solids are too strong to single out only one dominating band.

That being said, the extension of the single-band Hubbard model to the multi-band case is in order. As discussed in the last section, the hopping part is not hard to generalize. One only needs to enlargen the hopping matrix by further intra- and inter-orbital entries in the form of eq. (4). On the other hand, the interacting part is not quite that trivial to modify, since it amounts to generalize the quantum-chemical problem to a multi-orbital one in a given crystal field. The first thing to realize is that even when restricting to sole on-site interactions, according to eqs. (3,5) more Coulomb integrals and associated interactions now come into play. Immediately the question arises how to choose/compute the additional Coulomb parameters/functions in a certain crystal field. Since a deeper discussion of this (especially when accounting for the various symmetry issues) is rather involved and because many issues are still current line of research, we choose to discuss only briefly the model cases of e_g, t_{2g} and full p-, d- or f-shell within a cu-
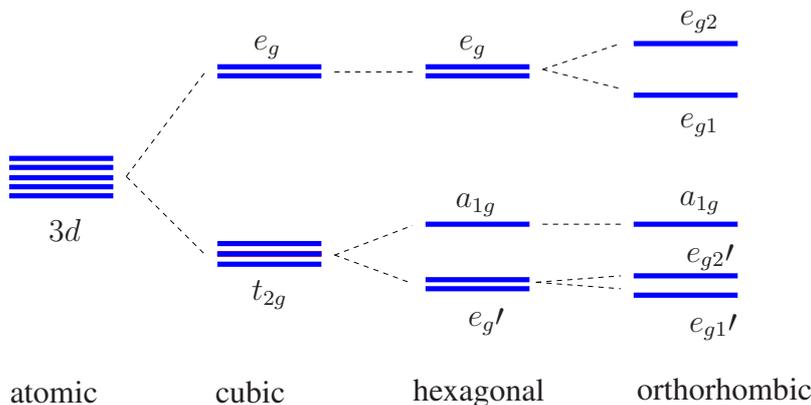
Fig. 4: *Splitting of the d-states in different crystal fields.*
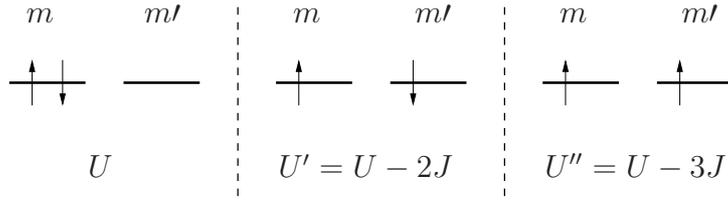
Fig. 5: *Local Coulomb interaction between two orbitals with enforcing Hund's first rule.*

bic crystal field. Some concrete results for the individual models will thereby be postponed to section 5 where we discuss the slave-boson approach to the numerical solution.

Lets assume first a cubic crystal-field splitting such that the t_{2g} states are significantly lower in energy than the e_g states (cf. Fig. 4). Moreover, a low-spin scenario shall hold, i.e., the lower-lying t_{2g} states first become filled according to Hund's first rule and only after that the e_g levels start to accumulate electrons. Then the filling of eight electrons (e.g. Ni^{2+}), because of the full t_{2g} subshell, poses in a good approximation the problem of two interacting electrons in the two e_g states. In a different case where the filling amounts to only four electrons (e.g. Ru^{4+}), one deals with a three-orbital problem composed of the t_{2g} manifold. The appropriate interacting lattice problem may be formulated in both cases as a generalized rotationally invariant multi-band Hubbard Hamiltonian through [20–22]

$$H_{\text{cub}} = \sum_{ij,mm',\sigma} t_{ij}^{mm'} c_{im\sigma}^{\dagger} c_{jm'\sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow} + \frac{1}{2} \sum_{i,m \neq m',\sigma} [U' n_{im\sigma} n_{im'\bar{\sigma}} + U'' n_{im\sigma} n_{im'\sigma}]$$
$$+ \frac{1}{2} \sum_{m \neq m',\sigma} \left[J c_{im\sigma}^{\dagger} c_{im'\bar{\sigma}}^{\dagger} c_{im\bar{\sigma}} c_{im'\sigma} + J_{\text{C}} c_{im\sigma}^{\dagger} c_{im\bar{\sigma}}^{\dagger} c_{im'\bar{\sigma}} c_{im'\sigma} \right] \quad . \tag{15}$$

It is seen that the complexity has quite increased compared to the single-band form (6), mainly due to the necessity of including the on-site exchange integral J. At this point its instructive to compare the exact expression for U and J derived from the general form (5).

$$U_{mm'} = \int d\mathbf{r} d\mathbf{r}' \, \varphi_{\mathbf{R}m\sigma}^{*}(\mathbf{r}) \, \varphi_{\mathbf{R}m'\sigma'}^{*}(\mathbf{r}') \, \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \, \varphi_{\mathbf{R}m'\sigma'}(\mathbf{r}') \, \varphi_{\mathbf{R}m\sigma}(\mathbf{r}) \quad , \tag{16}$$

$$J_{mm'} = \int d\mathbf{r} d\mathbf{r}' \, \varphi_{\mathbf{R}m\sigma}^{*}(\mathbf{r}) \, \varphi_{\mathbf{R}m'\sigma'}^{*}(\mathbf{r}') \, \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \, \varphi_{\mathbf{R}m\sigma'}(\mathbf{r}') \, \varphi_{\mathbf{R}m'\sigma}(\mathbf{r}) \quad . \tag{17}$$

Thus in principle these two Coulomb integrals are matrices that depend on the orbital indices m, m'. In a model spirit it proves however sufficient for the present symmetry to perform an orbital-independent parametrization, yet differentiating between intra- and inter-orbital terms. The intra-orbital Coulomb interaction shall be given by U and the inter-orbital Coulomb inter-actions by $U'=U-2J$ for different spin and $U''=U-3J$ for identical spin. Obviously, therewith Hund's first rule is correctly incorporated (see Fig. 5). In eq. (15) the terms in U, U' and U'' are *density-density interactions*, i.e., they can be written as products of particle-number operators. The remaining two terms in the second line of eq. (15) may not be written in this form, but are important to establish the full orbital rotational invariance of the Hamiltonian. These inter-actions are related to spin-flip and pair-hopping processes as can be verified by inspection. In

principle, the pair-hopping Coulomb integral J_C may be different than the one for the spin-flip term. However usually both interaction integrals are chosen to be equally identified with the exchange integral J. Remember again that the form of the model Coulomb integrals in eq. (15) is usually tailored to cubic symmetry. However in practice this structure for the multi-band Hamiltonian is also successfully applied in lower-symmetry cases (e.g. [23]).

Note that the given multi-band Hamiltonian may for the three-orbital t_{2g} problem also be written in a different way (but mathematical equivalent form) as

$$H_{\text{t2g}} = \sum_{ij,mm',\sigma} t_{ij}^{mm'} c_{im\sigma}^{\dagger} c_{jm'\sigma} + \frac{(U - 3J)}{2} N(N-1) + \frac{5}{2} JN - 2JS^2 - \frac{1}{2} JL^2 \quad , \quad (18)$$

with the total operators for particle number N, spin S and angular momentum L. This form is furthermore most often used in the context of a correlated p shell.

In the case of a full d- or f-shell there are even more complicated terms appearing in the derivation of the atomic Hamiltonian. In order to again establish complete rotational invariance, one best relies on the general form for local interactions

$$H_{\text{d}} = \sum_{ij,mm',\sigma} t_{ij}^{mm'} c_{im\sigma}^{\dagger} c_{jm'\sigma} + \frac{1}{2} \sum_{i,mm'm''m''',\sigma\sigma'} U_{mm'm''m'''} c_{im\sigma}^{\dagger} c_{im'\sigma'}^{\dagger} c_{im'''\sigma'} c_{im''\sigma} \quad . \quad (19)$$

The interaction matrix element can then be evaluated through a multipole expansion into effective Slater integrals F_k via

$$U_{mm'm''m'''} = \langle mm' | V_{ee}^{\text{loc}} | m'''m'' \rangle = \sum_{k=0} a_k(m, m', m'', m''') F_k \quad . \quad (20)$$

In a spherical approximation, only a finite number of Slater-integral terms form the sum and those are related to U and J. Then $U = F_0$ always holds and the further relations for the different ($l > 0$)-shells are usually chosen as follows

$$
\begin{aligned}
l = 1 \quad &: \quad J = \frac{1}{5} F_2 \quad , \\
l = 2 \quad &: \quad J = \frac{1}{14}(F_2 + F_4) \ , \ F_4 = 0.625 F_2 \quad , \\
l = 3 \quad &: \quad J = \frac{1}{6435}(286 F_2 + 195 F_4 + 250 F_6) \ , \ F_4 = 0.668 F_2 \ , \ F_6 = 0.494 F_2 \ .
\end{aligned}
\quad (21)
$$

Note that in current research there is nowadays the option to directly compute the necessary screened Coulomb integrals for a certain material system from approximated first-principles schemes, but this is beyond the scope of the present chapter.

Without going into the details of the multi-orbital models properties, lets just note that in the fully degenerate case the simple Mott scenario still applies, i.e., at integer filling the multi-band system can undergo a Mott transition. This means that e.g. for a three-band problem one may have an MIT for $n=1,2$.

3.3   More interactions

So far we only dealt with local Coulomb interactions in our model Hamiltonians, which may be indeed sufficient in the context of this school and as a good starting point. However of course, there are also limits to this kind of interaction, even when working in a multi-orbital scenario. Since nature does not care so much about the taste and wellness of theoretical physicists, eventually there are materials problems that ask for more.

For instance, one may easily think of problems where inter-site Coulomb interactions are not negligible anymore. In low-dimensional systems, especially quasi-1D compounds, the NN Coulomb integral V is often relevant at specific fillings to drive e.g. charge-density-wave (CDW) or spin-density-wave (SDW) instabilities [24]. The *extended Hubbard Hamiltonians* that are used for such modelings look like

$$H_{\mathrm{hubex}} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \varepsilon_0 \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{ij\sigma\sigma'} V_{ij} n_{i\sigma} n_{j\sigma'} \quad . \tag{22}$$

Most often the density-density interaction associated with V_{ij} is restricted to NN, but in principle the treatment of long-range Coulomb terms is possible.

Another action, retrieved from the collection of all possible pair interactions (see e.g. [6]) that may be relevant in some materials cases [25] is the so-called *correlated hopping* process with the interaction integral X. The associated Hamiltonian term has the following basic structure

$$H_{\mathrm{ch}} = \sum_{ij\sigma} X_{ij} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) (n_{i\bar{\sigma}} + n_{j\bar{\sigma}}) \quad . \tag{23}$$

Since the term within the first braces has the form of a bond-charge operator when summed over σ, the Hamiltonian H_{ch} may be interpreted as a bond-charge-site-charge repulsion [6].

Finally, the reserach area of model Hamiltonians also opens a route to go beyond the initial Born-Oppenheimer approximation. Remember that the BOA was introduced to decouple electronic and lattice degrees of freedom. However in many materials (e.g. manganites [26]) the electron-phonon coupling is significant and the BOA breaks down. Then there is the possibility to formulate a simplified Fröhlich Hamiltonian in real space using further only Einstein phonons, the so-called *Holstein Hamiltonian* [27]

$$H_{\mathrm{hol}} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - g \sum_{i\sigma} n_{i\sigma} \left(b_i^{\dagger} + b_i \right) + \omega \sum_{i} b_i^{\dagger} b_i \quad , \tag{24}$$

where $b^{(\dagger)}$ are bosonic creation/annihilation operators for the phonons, ω the Einstein-mode frequency and g the electron-phonon coupling strength.

There are many more model Hamiltonian approaches to specific microscopic processes. Note that for instance spin-orbit coupling was always excluded in our considerations, though the interplay of this phenomenon with Coulomb correlations is becoming a very active line of theoretical research (e.g. [19]). However this would here go beyond the scope of an elementary introduction to the field. We therefore now end the first part of this chapter of introducing basic model hamiltonians and turn to an, again brief, account of simpler theoretical methodolgies to actually put us in position to compute some of the discussed models properties.

4 Basic approaches to the single-band Hubbard model

In this first section of techniques to approach Hubbard-like models we deal with two traditional methodologies. We first discuss the standard mean-field framework of Hartree-Fock in the present model context. The second subsection introduces the simplest Green's-function based ansatz to the problem of locally interacting electrons, namely the so-called Hubbard-I approach. There are numerous excellent reviews of these basic approaches, e.g. [4,6,10], and its somehow a thankless task to add something to that in this short overview. Thus we will not challenge to confuse the reader by trying something terribly fancy but instead provide the necessary information in a nutshell along the lines of the already existing literature.

4.1 Hartree-Fock

When facing an interacting problem it is usually a very good idea to start with a mean-field approach, since it is simple but, importantly, non-trivial. Albeit nowadays many rather sophisticated techniques are available, one should never forget about the power and successes of mean-field (MF) theory.

Remember your quantum-mechanics class on many-particle wave functions in first quantization. Back then the simplest idea was to assume the full wave function may be decoupled and represented as a product of single-particle wave functions. After inserting in the Schrödinger equation, in the end every individual particle is moving in the *mean-field* build up by the other ones. Let us try to translate and apply this idea to the single-band Hubbard model in the form

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad . \tag{25}$$

Instead of applying a decoupling on the *states*, it is in the present context more efficient to decouple already on the *operator* level. Therefore we write the particle-number operator as

$$n_{i\sigma} = \langle n_{i\sigma} \rangle + \delta n_{i\sigma} \quad , \tag{26}$$

which means that there is a bulk part of $n_{i\sigma}$, its expectation value and hence a c-number, that accounts for the major observable physics. And a smaller part $\delta n_{i\sigma}$ that carries the still essential quantum-fluctuating nature around that. Neglecting the latter would be a bad idea, because this would lead to rather trivial results. Better write the interaction kernel therewith now as

$$n_{i\uparrow} n_{i\downarrow} = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \langle n_{i\downarrow} \rangle \delta n_{i\uparrow} + \langle n_{i\uparrow} \rangle \delta n_{i\downarrow} + \delta n_{i\uparrow} \delta n_{i\downarrow} =: A(n_{i\uparrow} n_{i\downarrow}) + \delta n_{i\uparrow} \delta n_{i\downarrow} \quad . \tag{27}$$

A similar analytical structure is obtained, i.e., the kernel separates into a, supposingly, bulky part and a smaller product of the fluctuations. Now we peform the approximation and neglect the *correlation of fluctuations* $\delta n_{i\uparrow} \delta n_{i\downarrow}$, which is at the heart of MF theory on the microscopic level. By eliminating $\delta n_{i\sigma}$ the Hubbard term hence reads

$$U \sum_i n_{i\uparrow} n_{i\downarrow} \approx U \sum_i A(n_{i\uparrow} n_{i\downarrow}) = U \sum_i \left(n_{i\uparrow} \langle n_{i\downarrow} \rangle + n_{i\downarrow} \langle n_{i\uparrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \right) \quad . \tag{28}$$

So within this approximation the tough interaction part looks rather harmless, merely equal to the particle-number operator with a site- and spin-dependent mean field. However before even examining details of this MF approach, one easily sees that something dramatic has happened to symmetry. The original spin rotational invariance of the Hubbard model is gone, since the MF interacting part can be rewritten using only the z component of the spin operator, i.e., $S_i^z = 1/2(n_{i\uparrow} - n_{i\downarrow})$. It is in fact a very important issue to understand that even if one uses the $(\uparrow, \downarrow)$ spin-projection basis in Fock space for the operator representation, the Hubbard term is still spin-rotational invariant. In some sense, our present MF approach shows the Hartree term but lacks its Fock companion.

The problem is that in eq. (27) we have unconsciously made a particular choice for decoupling the Hubbard term into a sum of simpler terms by singling out the particle-number operators. But the Hubbard model is more clever than that. In fact based on Wick's theorem a certain composition of operators can always be decoupled by forming all possible creation-annihilation pairs. Thus here

$$
\begin{aligned}
n_{i\uparrow} n_{i\downarrow} = c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} = - c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\uparrow} c_{i\downarrow} \quad \rightarrow \quad &- \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle c_{i\downarrow}^\dagger c_{i\uparrow} - \langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle c_{i\uparrow}^\dagger c_{i\downarrow} \\
&+ \langle c_{i\uparrow}^\dagger c_{i\uparrow} \rangle c_{i\downarrow}^\dagger c_{i\downarrow} + \langle c_{i\downarrow}^\dagger c_{i\downarrow} \rangle c_{i\uparrow}^\dagger c_{i\uparrow} \\
&+ \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle \langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle - \langle c_{i\uparrow}^\dagger c_{i\uparrow} \rangle \langle c_{i\downarrow}^\dagger c_{i\downarrow} \rangle \quad .
\end{aligned}
\tag{29}
$$

We easily identify the bulky A part of eq. (27) in there, but there is obviously a similar part stemming from the combinations $c_{i\downarrow}^\dagger c_{i\uparrow} =: S_i^+$ and $c_{i\downarrow}^\dagger c_{i\uparrow} =: S_i^-$. However this is just what we were looking for, as the spin-ladder operators should be capable to restore the spin-rotational invariance. Indeed bringing the former Hartree and this new Fock part together, the Hartree-Fock (HF) approximation to the Hubbard model can be cast into [6]

$$
H_{\text{hub}}^{\text{HF}} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_i \left\{ n_i \langle n_i \rangle - 4\mathbf{S}_i \langle \mathbf{S}_i \rangle - \frac{1}{2} \langle n_i \rangle^2 - 2 \langle \mathbf{S}_i \rangle^2 \right\} \quad ,
\tag{30}
$$

with $n_i = \sum_\sigma n_{i\sigma}$. At a first glance the interaction part looks more complicated, but note that it is only a single-particle term with a somewhat more sophisticated mean field. The approximate dispersion $\varepsilon_{\mathbf{k}\sigma}^{\text{HF}}$ with interaction is readily computed from (30) by e.g. choosing $\hat{e}_z$ as the quantization axis, transforming to k-space and using the identity $\sum_i n_{i\sigma} = \sum_{\mathbf{k}} n_{\mathbf{k}\sigma}$, which eventually leads to

$$
\varepsilon_{\mathbf{k}\sigma}^{\text{HF}} := \frac{\partial E_{\text{hub}}^{\text{HF}}}{\partial \langle n_{\mathbf{k}\sigma} \rangle} = \frac{\partial \langle H_{\text{hub}}^{\text{HF}} \rangle}{\partial \langle n_{\mathbf{k}\sigma} \rangle} =
\begin{cases}
\varepsilon_{\mathbf{k}} + U \left(\dfrac{n}{2} - m \right) & \text{for } \sigma = \uparrow \\[2mm]
\varepsilon_{\mathbf{k}} + U \left(\dfrac{n}{2} + m \right) & \text{for } \sigma = \downarrow
\end{cases}
\quad ,
\tag{31}
$$

with $m = 1/2(\langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle)$. Thus Hartree-Fock reveals the expected *exchange splitting* between spin-polarized bands in the ferromagnetic phase. Though HF is a weak-coupling approach to the Coulomb-interacting problem[8], due to the lack of screening it is ill-defined for metals (see e.g. [11]). In fact in some sense it is suited for *long-range ordered* Mott insulators, when

---

[8]HF only accounts for the first-order terms in the proper many-body diagrammatic perturbation theory for the interacting electron system (see e.g. [33]).
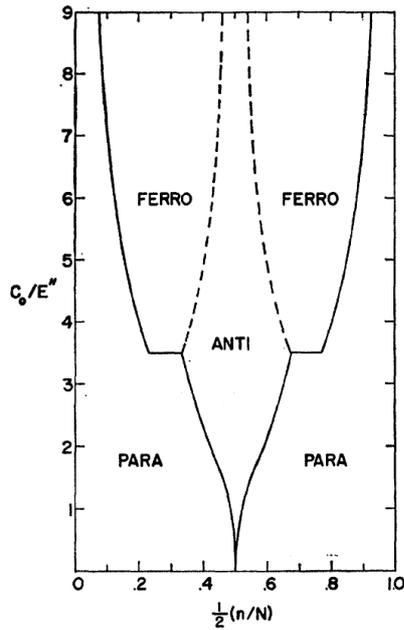
Fig. 6: *Normalized U-n Hartree-Fock phase diagram of the 3D Hubbard model on a simple cubic lattice taking paramagnetic, ferromagnetic and antiferromagnetic phases into account. Solid/Dashed lines indicate continuous/first order phase transitions. From [29].*

the charge gap can be described in the HF appoximation via an U-driven exchange gap (cf. eq. (31)). The so-called *LDA+U method* [28] makes explicit use of that in the context of first-principles calculations.

Equipped with this approximation one can nonetheless then start to study the competition between different phases like CDW, SDW, etc. But it is important to realize that the HF approximation may not account for explicit many-body effects such as e.g. band narrowing, finite lifetimes, or even a clear notion of Hubbard bands in the spectral function.

A magnetic phase diagram with taking NN collinear orderings into accout is shown in Fig. 6. Non-surprisingly increasing U seems to trigger magnetic order. As expected close to half filling and larger U an antiferromagnetic phase is stabilized due to superexchange. However a closer inspection shows that for $U \to \infty$ there will be competition also with the ferromagnetic phase. This is condensed in the Nagaoka theorem [30], stating that on many lattices at $U \to \infty$ the state with a single hole is indeed ferromagnetic. The whole issue of stabilizing ferromagnetic order in the Hubbard model is in fact far from being trivial (see e.g. [31,6] for a discussion). Note that since especially close to phase transitions the MF approximation of neglecting the correlation of fluctuations can be dangerous, one should keep in mind that there may be various changes to the HF phase diagram when using a more elaborate technique (as e.g. in [32]). Furthermore, incommensurate magnetic phases not displayed in Fig. 6 also have to be considered.

At this point some readers may still show some scepticism about the uniqueness of the decoupling exhibited in eq. (29). For instance one knows from the solid-state physics lecture that a metal may be unstable against pairing, i.e., forming a superconducting state. Obviously the shown decoupling is not capable of supporting such a phase, yet there is no a priori reason why the full Hubbard model should display the same insufficiency. And indeed, there are still more ways of decoupling the inconspicuous Hubbard term, e.g. allowing also for a superconducting amplitude (see [6]). Just think of the possibility of transforming the electron operators into

other bases and then redoing the decoupling. It is in the end once more some kind of "magic" of quantum mechanics that the simple-looking Hubbard model bears so much physics in it.

4.2 Hubbard I

At the introduction of the Hartree-Fock method we made reference to the derivation in the wave-function picture. Besides directly manipulating the operator terms as in the last section, one can also make direct use of other kind of representations in many-body physics, namely *many-particle Green's functions*[9]. The formal definition of the one-particle Green's function is given by

$$G_\sigma(\mathbf{R}_\alpha, t; \mathbf{R}_{\alpha'}, t') = -i\langle \Psi_0 | c_{\mathbf{R}_\alpha \sigma}(t) c^\dagger_{\mathbf{R}_{\alpha'}\sigma}(t') | \Psi_0\rangle \quad , \tag{32}$$

where the Heisenberg representation of the fermionic operators is important. The physical picture behind it is in principle simple. This function takes notes of the life of a created electron at spacetime $(\mathbf{R}_{\alpha'}, t')$ on top of the many-particle ground state $|\Psi_0\rangle$ until its death at spacetime $(\mathbf{R}_\alpha, t)$, asking for the probability to end up in the very same $|\Psi_0\rangle$. In a periodic solid its of course useful to Fourier transform this function to $(\mathbf{k}, \omega)$-space by invoking translational invariance and the explicit time independence of our Hamiltonian. The recorded information can then be read out in spectral form via the Lehmann representation [34]

$$G_\sigma(\mathbf{k}, \omega) = \sum_m \frac{|\langle \Psi_m^{(N_e+1)} | c^\dagger_{\mathbf{k}\sigma} | \Psi_0\rangle|^2}{\omega + \mu - \omega_{m0} + i\eta} + \sum_m \frac{|\langle \Psi_m^{(N_e-1)} | c_{\mathbf{k}\sigma} | \Psi_0\rangle|^2}{\omega + \mu - \omega_{0m} - i\eta} \quad , \tag{33}$$

where μ denotes the chemical potential. We can benefit from having introduced already the spectral function $A_\sigma(\mathbf{k}, \omega)$ in eq. (7) and write this in a more condensed form as an integral[10]

$$G_\sigma(\mathbf{k}, \omega) = \int_{-\infty}^\infty d\omega' \frac{A_\sigma(\mathbf{k}, \omega)}{\omega + \mu - \omega' + \mathrm{sgn}(\omega')i0^+} \quad . \tag{34}$$

For instance, taking the Fermi-gas limit from section 2.3, one immediately obtains

$$G_\sigma^{\mathrm{FG}}(\mathbf{k}, \omega) = \int_{-\infty}^\infty d\omega' \frac{\delta(\omega' - \varepsilon_\mathbf{k})}{\omega + \mu - \omega' + \mathrm{sgn}(\omega')i0^+} = \frac{1}{\omega + \mu - \varepsilon_\mathbf{k} + i\eta_\mathbf{k}} \quad . \tag{35}$$

with $\eta_\mathbf{k} = \mathrm{sgn}(|\mathbf{k}| - k_F)$. The power of the one-particle Green's function is build on the fact that it has complete record of the one-particle correlations of the system and allows, e.g., also to compute the expectation value of any single-particle operator, such as the total energy. In general it can be compactly rewritten as

$$G_\sigma(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \varepsilon_\mathbf{k} - \Sigma_\sigma(\mathbf{k}, \omega)} \quad , \tag{36}$$

where the *self-energy* $\Sigma_\sigma(\mathbf{k}, \omega)$ carries all deviations from the Fermi-gas limit due to Coulomb interactions[11]. Note that the self-energy is a true complex function and accounts therefore also for lifetime effects (e.g. such as we pointed out in section 2.3).

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[9]An excellent intoduction to this framework of theoretical many-body physics is e.g. given in [33].

[10]Note that going to an integral representation is only allowed in the large-N_e limit since it bears deeper physics about the excitations (see appendix H of [33]).

[11]The Pauli principle is usually enforced by hand in the Fermi gas, but Σ includes also the Fock term.

Lets try to compute also the Green's function in the atomic limit of the Hubbard model. Since the problem is separable we can limit the concentration on the local part of the Green's function, i.e., $G_{i\sigma}(\omega) = \sum_{\mathbf{k}} G_\sigma(\mathbf{k}, \omega)$ and insert in (34) the result (9) to reveal

$$
\begin{aligned}
G_{i\sigma}(\omega) &= \int_{-\infty}^0 d\omega' \frac{(1 - \langle n_{i\bar\sigma} \rangle)\, \delta(\omega' - \varepsilon_0)}{\omega + \mu - \omega' - i0^+} + \int_0^\infty d\omega' \frac{\langle n_{i\bar\sigma} \rangle\, \delta(\omega' - (\varepsilon_0 + U))}{\omega + \mu - \omega' + i0^+} \\
&= \frac{1 - \langle n_{i\bar\sigma} \rangle}{\omega + \mu - \varepsilon_0 - i0^+} + \frac{\langle n_{i\bar\sigma} \rangle}{\omega + \mu - \varepsilon_0 - U + i0^+} \quad .
\end{aligned}
\tag{37}
$$

Thus the former δ-Peak excitations are easily identified as the poles of the atomic Green's function. In order to extract the corresponding self-energy we have to bring it in the form of eq. (36). For simplicity we assume once again $\varepsilon_0 = 0$ and aim at the analytic structure

$$
G_{i\sigma}(\omega) = \frac{1}{\omega + \mu - \Sigma_{i\sigma}^{\mathrm{atom}}(\omega)} \quad ,
\tag{38}
$$

since no k-dependence should emerge. One readily realizes that the following form for the self-energy does the job:

$$
\Sigma_{i\sigma}^{\mathrm{atom}}(\omega) = U n_{i\bar\sigma} + U^2 \frac{n_{i\bar\sigma}(1 - n_{i\bar\sigma})}{\omega + \mu - U(1 - n_{i\bar\sigma})} \quad .
\tag{39}
$$

Albeit somewhat artificial, this representation opens the door to a first true many-body approximation compared to the effective single-particle HF treatment in mean field discussed in the last section. Because we can now make the radical assumption that the *true* self-energy of the solid shall have the analytical form of the atomic self-energy (39). This defines the so-called Hubbard-I (HI) approximation to the lattice Green's function, introduced in Hubbard's original paper [9], written as

$$
G_\sigma^{\mathrm{HI}}(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma_{i\sigma}^{\mathrm{atom}}(\omega)} \quad .
\tag{40}
$$

As usual the poles of $G_\sigma^{\mathrm{HI}}(\mathbf{k}, \omega)$ define the excitations. Inserting (39) in (40) and computing the roots of the denominator yields

$$
\varepsilon_{\mathbf{k}\sigma}^{\mathrm{HI}} = \frac{1}{2} \left\{ \varepsilon_{\mathbf{k}} + U \vee \pm \sqrt{(\varepsilon_{\mathbf{k}} + U)^2 + 4U \langle n_{i\bar\sigma} \rangle} \right\} \quad .
\tag{41}
$$

There are two solutions for each spin projection since there is, as already discussed in section 2.3, an upper and a lower Hubbard band. Hence whereas HF somehow approximates (with severe deficiencies) around the Fermi-gas limit, Hubbard I approximates around the atomic limit. Note that in HI the explicit Hubbard-band dispersion has k-dependent spectral weight $A_\sigma(\mathbf{k}, \omega)$, meaning that $\langle \Psi_{(m0)} | c_{\mathbf{k}\sigma}^{(\dagger)} | \Psi_{(m0)} \rangle$ now differs from one. This can be seen by bringing $G_\sigma^{\mathrm{HI}}(\mathbf{k}, \omega)$ in Lehmann form. But still, because the self-energy is a pure real object, no finite-lifetime effects are addressed in HI.

There are several further pros and cons of the HI approximation, for details see e.g. [10]. It is exact in the atomic limit as well as in the Fermi-gas limit (easily seen from eq. (41)), however it does not match the HF solution for small U. Furthermore perhaps the most important drawback

comes from the violation of particle-hole symmetry, which can be traced back to the use of *one* self-energy structure for the *two* Hubbard bands. In the end it is perhaps more the spirit of the approximation that renders the HI form rather relevant. On could think of a better approximate form of the local $\Sigma_{i\sigma}(\omega)$ in order to improve the method. This thought was indeed succesful and lead finally to the development of DMFT.

5 Slave-boson approach

In the last section of this brief introduction we aim to improve on the HF approximation by studying the true quasiparticle excitations in the strongly correlated metallic regime. This shall be done within a still simple but rather efficient technique with the politically incorrect naming slave-boson method. That approach shares its roots with the so-called *Gutzwiller approach* and both formalisms may in many cases be transformed into each other. However in the present text we will restrict the discussion to the slave bosons and provide references to some common and related initial work in this field [35–38]. More details on the nature of the performed approximation to the correlated problem may be also found in the review by Vollhardt [39] and references therein. Once again, the following presentation will be short and far from complete. It should mainly give the reader a first taste of the method.

5.1 Infinite-U limit

The general idea behind the Gutzwiller and the slave-boson method is given by the fact that electronic correlations impose certain constraints on the Hilbert space of available states of the problem. For instance its quite clear that in the context of the Hubbard model, double occupations on the lattice sites are severely surpressed at large U. Use of this was already made when writing down the t-J Hamiltonian for the limit $U/t \gg 1$ in section 2.3, where we explicitly projected onto (empty, single) occupied sites. However instead of "hard-coding" this effect in a new Hamiltonian form for a certain limit, one can also implement this physics in a more flexible way, giving rise to a new methodology for solving the actual Hubbard Hamiltonian.

In order to understand the basic principles of the approach it is instructive to first have look at the dispersive part of the single-band Hubbard model at $U \to \infty$, which we can write as

$$H = -t \sum_{\langle ij \rangle \sigma} P \, c_{i\sigma}^\dagger c_{j\sigma} \, P \quad , \tag{42}$$

whereby the projection P excludes the double occupied states $|\uparrow\downarrow\rangle$, leaving only the states $\{|0\rangle, |\sigma\rangle\}$ locally available (cf. Fig. 1). The question of course arises how to actually enforce this projection over the whole lattice in the calculation. In principle one has to demand that $\sum_\sigma n_{i\sigma} < 2$ on each site i. Recalling the standard lecture on Lagrange multipliers we however know that a constraint is usually best imposed via an *equality relation*. This can be formally achieved by introducing new auxiliary quantum degrees of freedom $\phi_i^{(\dagger)}$ such that we can de-

compose the original operators via

$$c_{i\sigma}^{\dagger} = f_{i\sigma}^{\dagger}\phi_i \qquad \wedge \qquad c_{i\sigma} = f_{i\sigma}\phi_i^{\dagger} \qquad . \qquad (43)$$

Since the $f_{i\sigma}^{(\dagger)}$ operators are still carrying the fermionic character, quantum mechanics teaches us that the $\phi_i^{(\dagger)}$ have to be of bosonic kind. The new operators are defined by their action and the corresponding particle-number-site statistics, i.e.,

$$
\begin{aligned}
\phi_i^{\dagger}|\text{vac}\rangle &= |0_i\rangle \quad, \\
f_{i\sigma}^{\dagger}|\text{vac}\rangle &= |\sigma_i\rangle
\end{aligned}
\qquad
\begin{aligned}
|0_i\rangle &: \quad n_b = 1 \quad \wedge \quad n_{f\sigma} = 0 \;, \\
|\uparrow_i\rangle &: \quad n_b = 0 \quad \wedge \quad n_{f\uparrow} = 1 \;, \\
|\downarrow_i\rangle &: \quad n_b = 0 \quad \wedge \quad n_{f\downarrow} = 1 \;,
\end{aligned}
\qquad (44)
$$

where $n_{f,b}$ denote the respective site occupation numbers and $|\text{vac}\rangle$ marks the vaccum state. Hence we now can truly formulate the necessary constraint on each lattice site i in the limit $U\to\infty$ as

$$\sum_\sigma f_{i\sigma}^{\dagger} f_{i\sigma} + \phi_i^{\dagger}\phi_i = 1 =: \mathcal{Q} \qquad (45)$$

and using the relations (43) we can directly choose to express the Hamiltonian form (42) in that limit via

$$H = -t \sum_{\langle ij\rangle\sigma} \phi_i\phi_j^{\dagger} f_{i\sigma}^{\dagger} f_{j\sigma} \qquad . \qquad (46)$$

In a simple picturing the decomposition of the physical electron operator $c_{i\sigma}^{(\dagger)}$ amounts here to a fragmentation into low-energy quasiparticle and high-energy Hubbard excitations on the operator level. The original operator takes care of both, the itinerant and the localized character of the electron, while $f_{i\sigma}^{(\dagger)}$ carries the sole quasiparticle part and the slave boson $\phi_i^{(\dagger)}$ only the high-energy remainings. Loosely speaking, the slave boson "releases" the electron from its high-energy excitations, which gives the political incorrectness a mild spin. However in detail things are truly a bit more complicated. As we have learned already in the HF subsection, such decouplings in quantum mechanics are seldom unique. In fact there is a gauge symmetry group associated with the redundancy of representing $c_{i\sigma}^{(\dagger)}$ via slave-boson techniques. The former manifests itself in the conservation of the pseudo charge $\mathcal{Q}$ defined in the constraint (45), thereby generating invariance under the group of local $U(1)$ gauge transformations (see e.g. [40, 13] and references therein for further details). This issue is interesting but drives us at presence a bit away from our simple goal of getting first concrete results for the Hubbard model, so lets get back to this.

Enforcing the constraint (45) on each lattice site individually is too tough, but in order to proceed it is a good idea to perform a MF approximation by condensing the bosons and averaging the constraint over all sites. We can then write

$$r := \langle\phi_i\rangle \quad , \qquad \sum_\sigma \langle n_{f\sigma}\rangle + |r|^2 = 1 \quad , \qquad H_{\text{eff}} = -|r|^2\, t \sum_{\langle ij\rangle\sigma} f_{i\sigma}^{\dagger} f_{j\sigma} \quad , \qquad (47)$$

with H_{eff} as the effective Hamiltonian in this slave-boson mean-field (SBMF) theory. In a functional-integral representation of the problem this approximation amounts to a saddle-point

approximation and therefore resembles the MF concept. Note that since $|r|^2=1-\langle n_f \rangle$ it also equals the doping δ away from half filling. Therewith one can define an effective hopping $t_{\text{eff}}=\delta t$ which provides readily the important Brinkman-Rice effect, namely that the quasiparticles become heavy (i.e., show small hopping amplitude) at small doping δ.

The ground state for finite chemical potential can then be found from minimizing the grand potential per lattice site

$$\Omega = \langle H_{\text{eff}} \rangle + \lambda \left(\sum_\sigma \langle n_{f\sigma} \rangle + |r|^2 - 1 \right) - \mu \sum_\sigma \langle n_{f\sigma} \rangle \tag{48}$$

with respect to the lagrange multiplier λ. In some sense the nature of the slave-boson technique is first to enlarge the Hilbert space by introducing additional bosonic degrees of freedom, which translates secondly in an enhancement of the variational freedom to select the actual physical states.

The quasiparticle dispersion is finally obtained from (48) via

$$\varepsilon_{\mathbf{k}\sigma}^{\text{SBMF}} := \frac{\partial E^{\text{SBMF}}}{\partial \langle n_{\mathbf{k}\sigma}^f \rangle} = |r|^2 \varepsilon_{\mathbf{k}\sigma} + \lambda \tag{49}$$

and the Green's function of the non-interacting fermionic quasiparticles hence reads

$$G_f(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}\sigma}^{\text{SBMF}}} = \frac{1}{\omega + \mu - |r|^2 \varepsilon_{\mathbf{k}} - \lambda} \quad . \tag{50}$$

However the one-particle Green's function of the true physical electrons results from inserting (43) in the definition (32) and using the MF approximation (47), i.e.,

$$G^{\text{SBMF}}(\mathbf{k}, \omega) = |r|^2 G_f(\mathbf{k}, \omega) = \frac{|r|^2}{\omega + \mu - |r|^2 \varepsilon_{\mathbf{k}} - \lambda} =: \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma^{\text{SBMF}}(\omega)} \quad . \tag{51}$$

The so defined local SBMF self-energy is then given by

$$\Sigma^{\text{SBMF}}(\omega) = \omega \left(1 - \frac{1}{|r|^2} \right) + \mu - \frac{\mu - \lambda}{|r|^2} \quad , \tag{52}$$

consisting of term linear in frequency ω and a static part. The latter accounts for a shift of the low-energy excitations and the former for the proper band renormalization. In fact $|r|^2$ if often named the quasiparticle weight Z, as for $Z=1$ one retrieves the Fermi-gas limit and $Z=0$ marks the vanishing of quasiparticle excitations. A value $0<Z<1$ therefore characterizes the so-called *Fermi-liquid regime*. As in HF, note that the Hubbard excitations do not appear in the associated spectral function, because we condensed the slave bosons. In principle Hubbard bands can be gained from treating fluctuations around the saddle-point, but this is a rather tricky issue (see e.g. [41]).

Although the slave-boson technique is approximate, we see that with already modest effort it can account for explicit many-body effects like the band-narrowing close to the Fermi level. But so far the method is not very useful for too many practical concerns, because we only dealt with the rather specific $U \to \infty$ case, mainly appropriate in the Kondo regime. However we would not have introduced the method here if there wasn't the possibility to extent it to the finite-U case, to be discussed next.

5.2 Kotliar-Ruckenstein representation

There are various options to extend the slave-boson method to finite U. Two prominent realization are the Kotliar-Ruckenstein (KR) representation [42] and the slave-rotor formalism [43]. In the following we briefly sketch the former methodology.

Somehow it is quite clear what is needed, since at finite U double occupations are of course still accessible one has to the extent the number of bosonic degrees of freedom in order to variationally cope with the enlarged number of lattice states. To study this without getting immediately lost in too many details, let us concentrate first on the slave-boson treatment of the simple atomic problem of a single correlated orbital [44]. The Hamiltonian for this Hubbard atom reads

$$H_{\text{loc}} = \varepsilon_0 \sum_\sigma c_\sigma^\dagger c_\sigma + U \, c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow \quad . \tag{53}$$

There are the already familiar four atomic states $\Gamma = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$ available for occupation. In the KR formalism one simply associates with *each* state a specific pair of slave-boson operators $\phi^{(\dagger)}$, i.e.,

$$\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\} \quad \rightarrow \quad \{\phi_0^{(\dagger)}, \phi_\uparrow^{(\dagger)}, \phi_\downarrow^{(\dagger)}, \phi_{\uparrow\downarrow}^{(\dagger)}\} \quad . \tag{54}$$

Since we are at finite U there is now no unique constraint on the actual occupation. However there are *two* new types of constraints which ensure that by enlarging the Hilbert space we truly recover in the calculation the physical electronic states based on the original $c_\sigma^{(\dagger)}$ operators. As there is no Pauli principle for bosons, we first have to demand that we only care about states with only a single slave boson, namely

$$\sum_\Gamma \phi_\Gamma^\dagger \phi_\Gamma = 1 \quad . \tag{55}$$

Secondly, the fermionic and bosonic content have to match in order to possibly recombine both parts to the actual physical electron, thus

$$\sum_\Gamma n_\sigma^\Gamma \, \phi_\Gamma^\dagger \phi_\Gamma = f_\sigma^\dagger f_\sigma \quad , \tag{56}$$

whereby n_σ^Γ marks the number of σ-electrons in the state Γ. We then *choose* to write the effective slave-boson Hamiltonian with the constraints already included as

$$H_{\text{loc}}^{\text{SB}} = \varepsilon_0 \sum_\sigma f_\sigma^\dagger f_\sigma + U \, \phi_{\uparrow\downarrow}^\dagger \phi_{\uparrow\downarrow} + \lambda_0 \left(\sum_\Gamma \phi_\Gamma^\dagger \phi_\Gamma - 1 \right) + \sum_\sigma \lambda_\sigma \left(\sum_\Gamma n_\sigma^\Gamma \, \phi_\Gamma^\dagger \phi_\Gamma - f_\sigma^\dagger f_\sigma \right) . \tag{57}$$

With the important choice of representing the single-particle part with the fermionic $f_\sigma^{(\dagger)}$ operators and the interacting term with the slave bosons $\phi_{\uparrow\downarrow}^{(\dagger)}$ we rendered the problem quadratic in the operators and therefore easily solvable. In order to do so, we do not even have to condense the bosons in our simple problem. It is possible to directly connect the finite-temperature
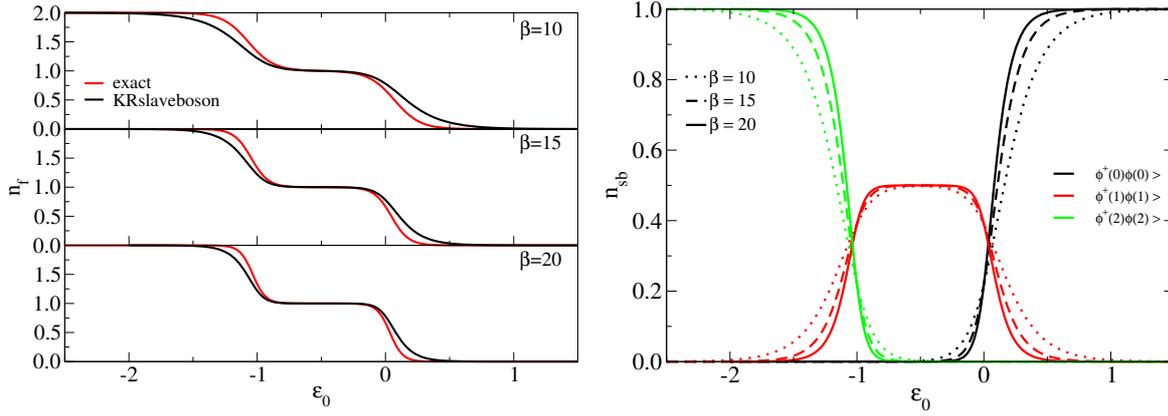
Fig. 7: *Hubbard atom within KR slave-boson theory. Left: Comparison with the exact result for the filling with level energy ε_0. Right: Individual level fillings from the slave-boson amplitudes.*

expectation values to the respective fermionic/bosonic distribution, namely

$$\langle f_\sigma^\dagger f_\sigma \rangle = n^{\mathrm{F}}(\varepsilon_0 - \lambda_\sigma) \quad , \quad \langle \phi_0^\dagger \phi_0 \rangle = n^{\mathrm{B}}(\lambda_0)$$
$$\langle \phi_\sigma^\dagger \phi_\sigma \rangle = n^{\mathrm{B}}(\lambda_0 + \lambda_\sigma) \quad , \quad \langle \phi_{\uparrow\downarrow}^\dagger \phi_{\uparrow\downarrow} \rangle = n^{\mathrm{B}}(U + \lambda_0 + \lambda_\uparrow + \lambda_\downarrow) \quad , \tag{58}$$

with $n^{\mathrm{B,F}}$ as the Bose-Einstein/Fermi-Dirac distribution functions. Therewith the constraints (55,56) read *on average*

$$n^{\mathrm{B}}(\lambda_0) + \sum_\sigma n^{\mathrm{B}}(\lambda_0 + \lambda_\sigma) + n^{\mathrm{B}}(U + \lambda_0 + \lambda_\uparrow + \lambda_\downarrow) - 1 = 0 \quad , \tag{59}$$

$$n^{\mathrm{B}}(U + \lambda_0 + \lambda_\uparrow + \lambda_\downarrow) + n^{\mathrm{B}}(\lambda_0 + \lambda_\sigma) - n^{\mathrm{F}}(\varepsilon_0 - \lambda_\sigma) = 0 \quad . \tag{60}$$

Aiming for a spin-unpolarized solution with $\lambda_\sigma = \lambda$, the above system of two nonlinear equations can be easily solved for (λ_0, λ). Note that the solution will be approximate, because the exact solution for the expectation value n_s for $s=0,1,2$ electrons on the model atom is of course given by

$$\langle n_s \rangle = \frac{\sum_\Gamma n_s^\Gamma \, e^{-\beta E_\Gamma}}{\sum_\Gamma e^{-\beta E_\Gamma}} \quad , \tag{61}$$

with E_Γ as the energy in state Γ according to the true Hamiltonian (53) and β the inverse temperature. Figure 7 shows the slave-boson solution along with the exact Coulomb staircase for different inverse temperatures.

The general application of the KR scheme is surely not concentrated on atomic problems, but of course on single- and multi-orbital Hubbard-like models on the lattice. In general its useful to increase formality and write the representation of the physical electron operator for a certain (site, orbital, spin projection) as (see e.g. [45] for details)

$$c_{im\sigma}^{\dagger(\mathrm{SB})} := \underline{c}_{im\sigma}^\dagger = r_{im}^*(\{\phi\}) f_{im\sigma}^\dagger = \sum_{pq} \langle p_i | f_{im\sigma}^\dagger | q_i \rangle \, \phi_{pi}^\dagger \phi_{qi} \, f_{im\sigma}^\dagger \quad . \tag{62}$$

Here $|p\rangle$, $|q\rangle$ mark the quasiparticle Fock states $f_{im\sigma}^{(\dagger)}$ is acting on. Its convenient to express the original physical states in the enlarged product Hilbert space of the quasiparticles and bosons
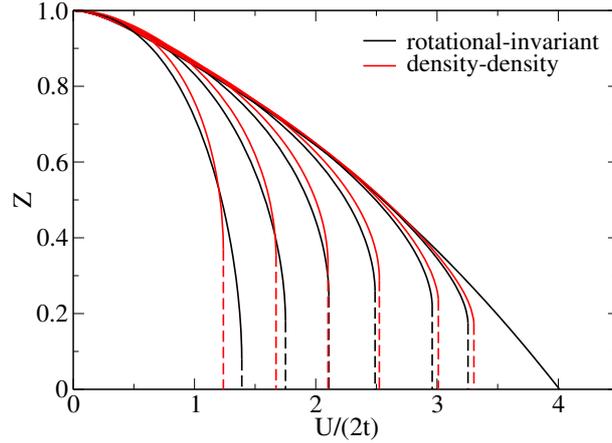
Fig. 8: *Quasiparticle weight Z versus U for the two-band Hubbard model on a 3D simple-cubic lattice, NN hopping and no inter-band hopping. Influence of $J=J_C$ on the Mott transition in calculations with and without spin-flip and pair-hopping terms at half filling ($n=2$) for equal bandwidths (from [45]). Right to left: $J/U=0,0.01,0.02,0.05,0.10,0.20,0.45$.*

therefore as

$$|\underline{p}_i\rangle := \phi_{pi}^{\dagger}|\mathrm{vac}_i\rangle \otimes |p_i\rangle_f \quad . \tag{63}$$

Note that we again only have one slave boson for the physical state, something that has again to be enforced via the constraint (55). The effective Hamiltonian for the single-band Hubbard model will then be given by

$$\underline{H}_{\mathrm{hub}} = -t \sum_{\langle ij\rangle\sigma} r_i r_j^* f_{i\sigma}^{\dagger} f_{j\sigma} + U \sum_i \phi_{\uparrow\downarrow i}^{\dagger} \phi_{\uparrow\downarrow i} \quad . \tag{64}$$

Throughout this equations for the quasiparticle and slave-boson operators the site index i is surely lost in the MF approximation most often applied in the actual calculations on the lattice. In that sense the conventional KR-SBMF theory is a local approach to correlations, i.e., no inter-site self-energy terms are revealed.

A serious drawback of the standard KR scheme is given by the fact that it can only be applied to density-density interactions. Therefore general multi-orbital Hamiltonians like (15) with spin-flip and pair-hopping terms can not be adequately treated. One can overcome this problem by further extending the framework to a rotationally invariant scheme [46,47,45,48,49]. However the details of that topic are beyond our brief introduction and we therefore close this section with just showing the rotationally invariant slave-boson result for the general two-band case of the Hamiltonian (15) at half filling in Fig. 8.

6 Final remarks

The goal of this chapter was to give readers that are new to the field a basic introduction to the theoretical research on model Hamiltonians in condensed matter physics. Those who have already or who will have a look at some of the literature referenced here will readily see that we

only scarcely scratched the tip of the iceberg associated with this topic. Nonetheless, the local viewpoint on electronic correlations, taken here for most of the Hamiltonians, and the basic techniques appear to be an appropriate starting point for many phenomena.

Concerning the techniques, the reader should clearly see that there is much room for improvement. Especially treating quasiparticles and Hubbard excitations on an equal footing appears, from what we have seen so far, to be tough. In the chapters to come we will realize how dynamical mean-field theory exactly cures this problem within an again local representation of the electronic self-energy. That is, however, still not the end of the story, there are and will be challenges where one eventually has to go beyond this, just think of long-range fluctuations close to (quantum) critical points.

When discussing the justification for model Hamiltonians compared to pure first-principles approaches in the introductory section of this chapter we already mentioned the reasons. But let us remember in the end once more that such models are excellent tools to single out the essential physical mechanisms in given problems without getting lost in too many, often irrelevant, details. In order to finally deal with emergent phenomena in physics one has to remember this thinking and one should therefore be strongly motivated not to forget it when working with modern first-principles(-like) approaches, as for instance provided by LDA+DMFT.

Acknowledgment

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