

# A 9    Electron Correlations

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In 1929 Dirac [1] noted that with the advent of quantum mechanics

The underlying laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that exact applications of these laws lead to equations which are too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

By now there is indeed a very successful such method: density functional theory (DFT), which was the subject of all the previous lectures [2]. Although in principle exact, in practice DFT is approximate since the exact density functional is not known. Nevertheless, density functional calculations provide an accurate *ab initio* description of wide classes of materials. They often fail, however, to capture, even qualitatively, the essential physics of systems with open *d* and *f* shells. Since the *d*- and *f*-orbitals are very localized, the Coulomb repulsion between the electrons is significant. When the Coulomb repulsion is large the electrons can no longer be described as moving independently. Instead the movement of one electron depends on the position of all the other electrons, since it has to avoid their Coulomb repulsion. The electrons are said to be *strongly correlated* and the picture of individual electrons breaks down.

Understanding the physics of strongly correlated systems is one of the central challenges of modern condensed-matter physics. In the present lectures we will focus on the simplest model for investigating correlations: the Hubbard model. In the first part we will show how we can understand magnetic exchange mechanisms based on a Hubbard model description. Since for this we need only consider very small systems, this will also serve as an introduction to the notation used to describe many-body systems and introduce you to the concept of a model Hamiltonian. It should also give you a first impression of how many-body wave-functions look like. Further on, we introduce the downfolding technique for eliminating high-energy degrees of freedom. In the second part we will consider the Hubbard model for extended systems. There we will in particular focus on the most striking correlation effect: the Mott transition. Moreover, using downfolding, we show how to derive the Heisenberg model from the Hubbard Hamiltonian. In the last part we give a brief introduction to the Lanczos method for the exact diagonalization of model Hamiltonians.

## 1 Exchange mechanisms

One of the surprises of the theory of magnetism is that magnetic ordering is normally *not* caused by magnetic interactions. Instead, magnetism in solids is mainly a manifestation of strong electron-electron interactions. Coupling between spins arises already in systems without explicit spin-spin interaction. It is a consequence of the competition between the kinetic energy of the electrons and their Coulomb repulsion, and, of course, the Pauli principle. An example known from atomic physics is Hund's rule: In an open shell spins align in parallel since then the Pauli principle helps to reduce their Coulomb repulsion. This mechanism is called *direct exchange*. It arises when calculating the matrix element of the Coulomb interaction for a Slater determinant. The resulting spin-spin interaction term is thus a direct consequence of the Pauli principle. In the following we will investigate indirect exchange mechanisms. They arise from higher-order processes and are obtained as effective terms in the Hamiltonian after eliminating states with large Coulomb energy.

## 1.1 Kinetic exchange

Our first goal is to understand how a spin-spin interaction can arise from a spin-independent Hamiltonian. For this we consider a simplified version of the calculation for the  $H_2$  molecule. We consider two (orthogonal) orbitals,  $\phi_1$  and  $\phi_2$ , separated by some distance. If we add an electron to the system, that electron will be able to move between the two orbitals, with a matrix element  $-t$ . Because we allow the electron to only occupy two orbitals, the Hamiltonian describing it is a  $2 \times 2$  matrix

$$H = \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix}. \quad (1)$$

This *tight-binding* Hamiltonian is easily diagonalized giving the linear combinations

$$\phi_{\pm} = \frac{1}{\sqrt{2}} (\phi_1 \pm \phi_2) \quad (2)$$

as eigenstates with eigenenergies  $\varepsilon_{\pm} = \mp t$ . The hopping matrix element is negative, which means that the state without a node,  $\phi_+$ , is the ground state.

Pictorially we can write the basis states by specifying which orbital the electron occupies. For a spin-up electron we then write

$$\phi_1 = |\uparrow, \cdot\rangle \quad \text{and} \quad \phi_2 = |\cdot, \uparrow\rangle \quad (3)$$

where we now represent the basis states by where the electron is located.

If there are two electrons in the system, i.e., one electron per orbital, then we can again use basis states which just specify, which orbital the electrons occupy. For two electrons of opposite spin we then find two states where the electrons are sitting in the same orbital

$$|\uparrow\downarrow, \cdot\rangle \quad |\cdot, \uparrow\downarrow\rangle \quad \text{“ionic states”}$$

and two states where the electrons are sitting in different orbitals

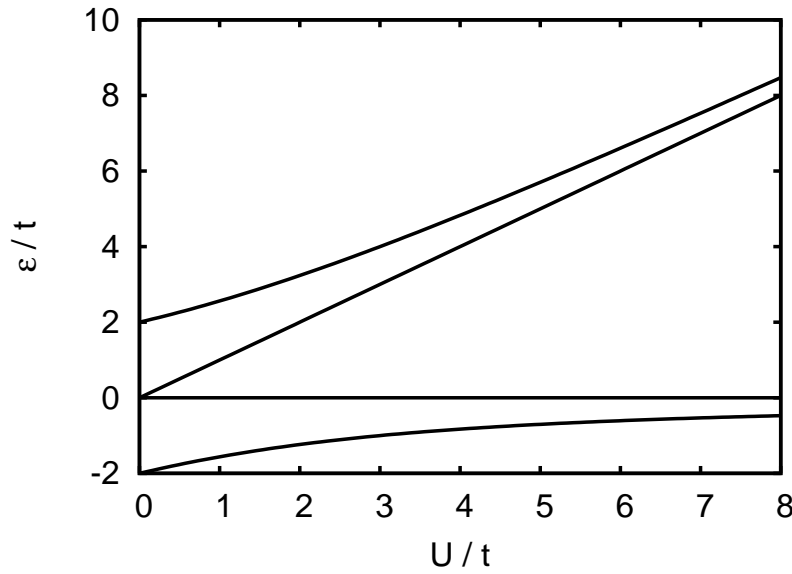
$$|\uparrow, \downarrow\rangle \quad |\downarrow, \uparrow\rangle \quad \text{“covalent states”}.$$

In this basis we can write the Hamiltonian matrix for our simple model of the  $H_2$  molecule as

$$H = \begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & +t & +t \\ -t & +t & U & 0 \\ -t & +t & 0 & U \end{pmatrix} \begin{matrix} |\uparrow, \downarrow\rangle \\ |\downarrow, \uparrow\rangle \\ |\uparrow\downarrow, \cdot\rangle \\ |\cdot, \uparrow\downarrow\rangle \end{matrix} \quad (4)$$

You should convince yourself that, indeed, hopping of a single electron connects covalent and ionic states, and that the sign changes are due to the transposition of the electrons (Fermion sign). In addition we introduce a matrix element  $U$  in the diagonal for states with two electrons in the same orbital to describe the Coulomb repulsion when the electrons are close to each other. Diagonalizing  $H$  we find the energy spectrum and the corresponding eigenstates:

$$\begin{aligned} \varepsilon_{\pm} &= \frac{U}{2} \pm \frac{\sqrt{U^2 + 16t^2}}{2}, & \Psi_{\pm} &= \frac{\left( |\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle - \frac{\varepsilon_{\pm}}{2t} [|\uparrow\downarrow, \cdot\rangle + |\cdot, \uparrow\downarrow\rangle] \right)}{\sqrt{2 + \varepsilon_{\pm}^2/(2t^2)}} \\ \varepsilon_{\text{cov}} &= 0, & \Psi_{\text{cov}} &= \frac{1}{\sqrt{2}} \left( |\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle \right) \\ \varepsilon_{\text{ion}} &= U, & \Psi_{\text{ion}} &= \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow, \cdot\rangle - |\cdot, \uparrow\downarrow\rangle \right) \end{aligned}$$



**Fig. 1:** Spectrum of the two-site Hubbard model as a function of  $U$ . For large  $U$  there are two levels with energy close to zero. Their energy difference corresponds to the exchange energy. The remaining two states with ionic character have an energy roughly proportional to  $U$ .

The eigenenergies as a function of  $U$  is shown in figure 1.

Now we consider the limit of  $U$  much larger than  $t$ , the large- $U$  limit. From figure 1 we see that there are two states with energies that increase with  $U$ . They are the states  $\Psi_{\text{ion}}$  and  $\Psi_{+}$  that have considerable contributions of the ionic states. Then there are two states whose energy is close to zero. They are the states that have mainly covalent character. To find the energy and the character of these levels in the limit  $U \rightarrow \infty$  we can just expand  $\epsilon_{-} \rightarrow -4t^2/U$  and  $\epsilon_{+} \rightarrow U - 4t^2/U$ . We thus see that while the purely covalent state  $\Psi_{\text{cov}}$  is independent of  $U$ ,  $\Psi_{-}$  has a slightly lower energy due to some small admixture of the ionic states. The latter state cannot be expressed, even approximately, as a Slater determinant. This is the reason why strongly correlated systems are so difficult to describe.

A more instructive method to analyze the limit of large  $U$ , which can easily be generalized to more complex situations, where we can no longer diagonalize the full Hamiltonian, is the downfolding technique. It is explained in the appendix. The idea of downfolding is to partition the Hilbert space into parts that are of interest, here the covalent type states, and states that should be projected out, here the ionic states. With this partitioning we can view the Hamiltonian matrix (4) as built of  $2 \times 2$  submatrices. Calculating the inverse on the space of covalent states (see equation 62 in the appendix) we find an *effective Hamiltonian* which now operates on the covalent states only:

$$H_{\text{eff}}(\epsilon) = \begin{pmatrix} -t & -t \\ +t & +t \end{pmatrix} \begin{pmatrix} \epsilon - U & 0 \\ 0 & \epsilon - U \end{pmatrix}^{-1} \begin{pmatrix} -t & +t \\ -t & +t \end{pmatrix} \approx -\frac{2t^2}{U} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad (5)$$

In the last step we have set  $\epsilon$  to zero.

The process of eliminating the ionic states thus gives rise to an effective interaction between the covalent states, which was not present in the original Hamiltonian (4). Diagonalizing the

effective Hamiltonian we find

$$\begin{aligned}\varepsilon_s &= -\frac{4t^2}{U} \quad , \quad \Psi_s = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \\ \varepsilon_t &= 0 \quad , \quad \Psi_t = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle)\end{aligned}$$

These states correspond to the singlet and triplet states in the hydrogen molecule. Here the singlet-triplet splitting is  $J = -4t^2/U$ . The other states in the triplet are those with two electrons of parallel spin:  $|\uparrow, \uparrow\rangle$  and  $|\downarrow, \downarrow\rangle$ . They, of course, also have energy zero, as hopping is impossible due to the Pauli principle.

To understand the nature of the effective interaction in the low-energy Hamiltonian we observe that the off-diagonal matrix elements in (5) correspond to flipping the spin of both electrons (“exchange”). Remembering that

$$\vec{S}_1 \cdot \vec{S}_2 = S_1^z S_2^z + \frac{1}{2} \left( S_1^+ S_2^- + S_1^- S_2^+ \right) \quad (6)$$

we see that the effective interaction will contain a spin-spin coupling term.

A more systematic way for obtaining the form of the effective interaction is by using second quantization, which will also help to simplify our notation. In *second quantization* we use operators to specify in which orbital an electron is located. As an example,  $c_{1,\uparrow}^\dagger$  puts a spin-up electron in orbital  $\phi_1$ . Denoting the system without electrons by  $|0\rangle$  the basis states that we have considered so far are thus written as

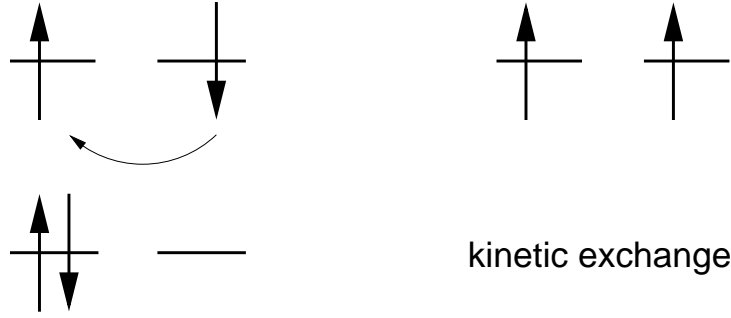
$$\begin{aligned}|\uparrow, \cdot\rangle &= c_{1,\uparrow}^\dagger |0\rangle \\ |\cdot, \uparrow\rangle &= c_{2,\uparrow}^\dagger |0\rangle \\ |\uparrow, \downarrow\rangle &= c_{2,\downarrow}^\dagger c_{1,\uparrow}^\dagger |0\rangle \\ |\downarrow, \uparrow\rangle &= c_{2,\uparrow}^\dagger c_{1,\downarrow}^\dagger |0\rangle \\ |\uparrow\downarrow, \cdot\rangle &= c_{1,\downarrow}^\dagger c_{1,\uparrow}^\dagger |0\rangle \\ |\cdot, \uparrow\downarrow\rangle &= c_{2,\downarrow}^\dagger c_{2,\uparrow}^\dagger |0\rangle\end{aligned}$$

In order to describe the hopping of an electron from one orbital to another, we introduce operators that annihilate an electron. For example  $c_{1,\uparrow}$  removes a spin-up electron from orbital  $\phi_1$ . The hopping of an up electron from  $\phi_1$  to  $\phi_2$  is thus described by the operator  $c_{2,\uparrow}^\dagger c_{1,\uparrow}$  that first takes an electron out of orbital 1 and then creates one in orbital 2. The Hamiltonian for a spin-up electron hopping between two orbitals can thus be written as

$$H = -t \left( c_{1,\uparrow}^\dagger c_{2,\uparrow} + c_{2,\uparrow}^\dagger c_{1,\uparrow} \right). \quad (7)$$

Calculating the matrix elements with the single-electron basis states we recover the matrix (1). For the calculation we need to know that the operators that describe the electrons *anticommute*. This reflects that a many-electron wave function changes sign when two electrons are exchanged. Using the notation  $\{a, b\} = ab + ba$  we have

$$\{c_{i\sigma}, c_{j\sigma'}\} = 0 \quad \{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0 \quad \{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{i,j} \delta_{\sigma,\sigma'}$$



**Fig. 2:** Simple picture of kinetic exchange: The antiparallel alignment of the spins is favored, since it allows the electrons to hop to the neighboring site.

Moreover, trying to annihilate an electron in a state where there is no electron results in zero:  $c_{i\sigma}|0\rangle = 0$ . Finally, as the notation implies,  $c_{i\sigma}^\dagger$  is the adjoint of  $c_{i\sigma}$  and  $\langle 0|0\rangle = 1$ .

To describe the Coulomb repulsion between two electrons in the same orbital we use that  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  returns 0 when operating on a basis state with no spin- $\sigma$  electron in orbital  $\phi_i$ , and has the eigenvalue 1 for a basis state with a spin- $\sigma$  electron in orbital  $\phi_i$ . It is thus called the occupation number operator. The Coulomb repulsion in orbital  $\phi_1$  is then described by the operator  $U n_{1\uparrow} n_{1\downarrow}$ , which is non-zero only when there is a spin-up *and* a spin-down electron in  $\phi_1$ . The Hamiltonian for our two-orbital model is thus given by

$$H = -t \left( c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\uparrow}^\dagger c_{1\uparrow} \right) + U \left( n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow} \right). \quad (8)$$

You should convince yourself that when you calculate the matrix elements for the two-electron states, you recover the matrix (4).

Coming back to the effective Hamiltonian (5), we can rewrite  $H_{\text{eff}}$  in second quantization.

$$H_{\text{eff}} = -\frac{2t^2}{U} \left( c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger c_{1\downarrow} c_{2\uparrow} - c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger c_{1\downarrow} c_{2\uparrow} - c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger c_{1\uparrow} c_{2\downarrow} + c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger c_{1\uparrow} c_{2\downarrow} \right) \quad (9)$$

$$= -\frac{2t^2}{U} \left( c_{1\downarrow}^\dagger c_{1\downarrow} c_{2\uparrow}^\dagger c_{2\uparrow} - c_{1\uparrow}^\dagger c_{1\downarrow} c_{2\downarrow}^\dagger c_{2\uparrow} - c_{1\downarrow}^\dagger c_{1\uparrow} c_{2\uparrow}^\dagger c_{2\downarrow} + c_{1\uparrow}^\dagger c_{1\uparrow} c_{2\downarrow}^\dagger c_{2\downarrow} \right) \quad (10)$$

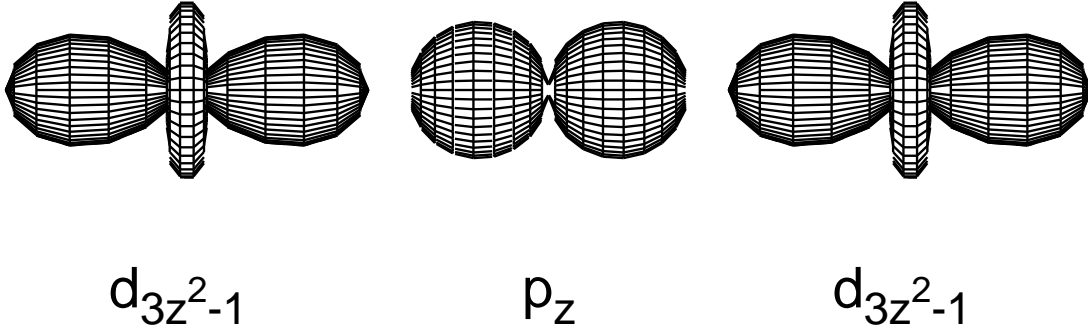
Looking at equation (56) in the appendix we see that the spin operators are given by

$$S_i^x = \frac{1}{2} \left( c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow} \right) \quad S_i^y = -\frac{i}{2} \left( c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow} \right) \quad S_i^z = \frac{1}{2} \left( n_{i\uparrow} - n_{i\downarrow} \right) \quad (11)$$

From this we find (after some calculation) that the effective Hamiltonian can be written in terms of the spin operators

$$H_{\text{eff}} = \frac{4t^2}{U} \left( \vec{S}_1 \cdot \vec{S}_2 - \frac{n_1 n_2}{4} \right) \quad (12)$$

To finish, we again stress that the completely spin-independent Hamiltonian (8), in the limit of large  $U$ , gives rise to a spin-spin interaction. Since the exchange coupling  $J = 4t^2/U$  is positive, states with antiparallel spins have lower energy. Thus kinetic exchange leads to *antiferromagnetism*. We, again, point out that the singlet-triplet splitting for the effective Hamiltonian really arises from the admixture of ionic states into the singlet. By downfolding we can eliminate the high-energy ionic states from our Hilbert space. The eliminated states then give rise to an effective spin-spin interaction on the new reduced low-energy Hilbert space. We must therefore keep in mind that when working with the effective Hamiltonian (12) we are considering different states than when working with the original Hamiltonian (8).



**Fig. 3:** In superexchange an oxygen  $p$  orbital mediates the exchange interaction between two transition-metal  $d$  orbitals.

## 1.2 Superexchange

For the kinetic exchange mechanism it is crucial that there is hopping between the orbitals. These orbitals are typically the very localized  $d$  orbitals of transition-metals. However, kinetic exchange cannot explain the antiferromagnetism of most transition-metal compounds: Since the  $d$  orbitals are so localized hopping can only occur between orbitals on different atoms, when these are very close to each other. But most antiferromagnetic insulators are transition-metal *oxides*, so that the transition-metal cations are separated by large oxygen anions. In such a situation, shown in figure 3, direct hopping between the  $d$  orbitals is very unlikely. The concept of kinetic exchange can, however, be extended to these cases by taking into account hopping via the intermediate  $p$  orbital. This mechanism is called superexchange.

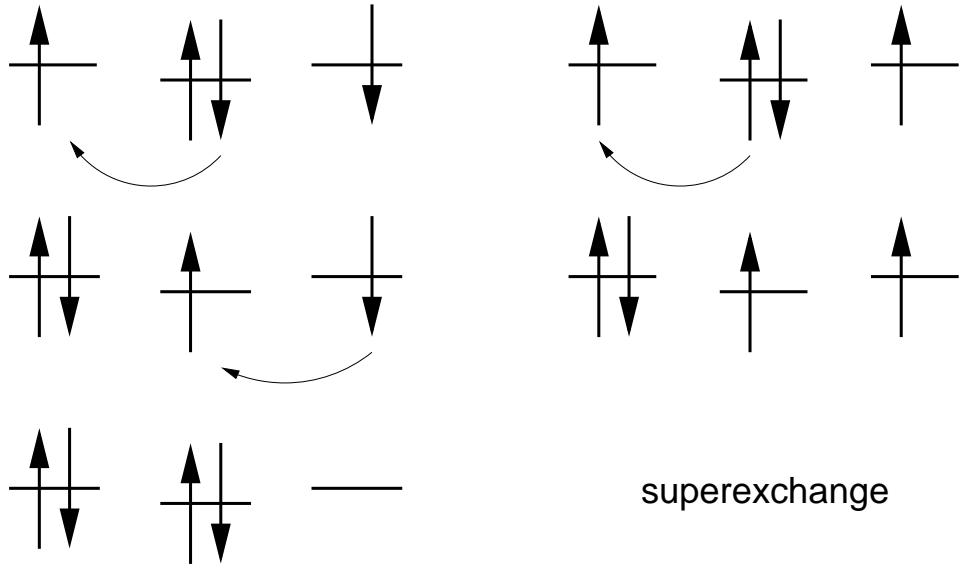
To understand superexchange, we consider two  $d$  orbitals with an extended oxygen  $p$  orbital in between. We introduce the operator  $c_{i\sigma}^\dagger$ , which creates a spin- $\sigma$  electron in  $d$  orbital at site  $i$ , where  $i = 1$  denotes the  $d$  orbital on the left and  $i = 2$  the one on the right (see figure 3). Likewise  $c_{p\sigma}^\dagger$  creates an electron in the  $p$  orbital. The energy of an electron in a  $d$  or  $p$  orbital is  $\varepsilon_d$  and  $\varepsilon_p$ , respectively. The Coulomb repulsion between two electrons in a  $d$  orbital is  $U_d$ , while we can neglect the repulsion between electrons in a  $p$  orbital, since the orbital is quite spread out and thus the repulsion is relatively small. Finally,  $-t_{pd}$  is the hopping between  $p$  and  $d$  orbitals. The Hamiltonian for the system of figure 3 is then given by

$$H = \sum_{\sigma} \left( \varepsilon_d \sum_i n_{i\sigma} + \varepsilon_p n_{p\sigma} - t_{pd} \sum_i \left( c_{i\sigma}^\dagger c_{p\sigma} + c_{p\sigma}^\dagger c_{i\sigma} \right) \right) + U_d \sum_i n_{i\uparrow} n_{i\downarrow} \quad (13)$$

In the absence of hopping, the ground state will have singly occupied  $d$  orbitals, corresponding to a positively charged transition-metal ion, and a doubly occupied  $p$  orbital, corresponding to an  $O^{2-}$  ion. To study a possible coupling between the spins on the  $d$  orbitals, we first look at the case, where both  $d$ -spins point upwards. The Hamiltonian matrix in the corresponding Hilbert space is then given by

$$H = \left( \begin{array}{c|cc} 0 & t_{pd} & t_{pd} \\ \hline t_{pd} & U_d - \Delta_{pd} & 0 \\ t_{pd} & 0 & U_d - \Delta_{pd} \end{array} \right) \begin{array}{l} c_{2\uparrow}^\dagger c_{p\downarrow}^\dagger c_{p\uparrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \\ c_{2\uparrow}^\dagger c_{p\uparrow}^\dagger c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \\ c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger c_{p\uparrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \end{array} \quad (14)$$

where we have chosen  $2(\varepsilon_p + \varepsilon_d)$  as the zero of our energy scale and defined  $\Delta_{pd} = \varepsilon_p - \varepsilon_d$ . The basis states of the Hilbert space are given on the right and the lines indicate the partitioning



**Fig. 4:** Simple picture of superexchange. Here the orbital on the central site is different from the orbitals on the sides. Typically in the center there is a oxygen  $p$  orbital coupling two  $d$  orbitals. This situation is illustrated in figure 3.

of the Hilbert space for downfolding. The effective Hamiltonian for parallel spins on  $d$  orbitals is then

$$H_{\text{eff}} = (t_{pd}, t_{pd}) \begin{pmatrix} \varepsilon - (U_d - \Delta_{pd}) & 0 \\ 0 & \varepsilon - (U_d - \Delta_{pd}) \end{pmatrix} \begin{pmatrix} t_{pd} \\ t_{pd} \end{pmatrix} \approx -\frac{2t_{pd}^2}{U_d - \Delta_{pd}} \quad (15)$$

where in the last step we have set  $\varepsilon$  to zero.

For antiparallel spins the Hilbert space is six-dimensional leading to the Hamiltonian matrix

$$\begin{pmatrix} 0 & 0 & t_{pd} & t_{pd} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{pd} & t_{pd} & 0 & 0 \\ \hline t_{pd} & 0 & U_d - \Delta_{pd} & 0 & 0 & 0 & -t_{pd} & 0 \\ t_{pd} & 0 & 0 & U_d - \Delta_{pd} & 0 & 0 & 0 & -t_{pd} \\ 0 & t_{pd} & 0 & 0 & U_d - \Delta_{pd} & 0 & t_{pd} & 0 \\ 0 & t_{pd} & 0 & 0 & 0 & U_d - \Delta_{pd} & 0 & t_{pd} \\ 0 & 0 & -t_{pd} & 0 & t_{pd} & 0 & U_d & 0 \\ 0 & 0 & 0 & -t_{pd} & 0 & t_{pd} & 0 & U_d \end{pmatrix} \begin{matrix} c_{2\downarrow}^\dagger c_{p\downarrow}^\dagger c_{p\uparrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \\ c_{2\uparrow}^\dagger c_{p\downarrow}^\dagger c_{p\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle \\ c_{2\downarrow}^\dagger c_{p\uparrow}^\dagger c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \\ c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger c_{p\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \\ c_{2\uparrow}^\dagger c_{p\downarrow}^\dagger c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \\ c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger c_{p\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle \\ c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger c_{p\downarrow}^\dagger c_{p\uparrow}^\dagger |0\rangle \\ c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger c_{p\uparrow}^\dagger c_{p\downarrow}^\dagger |0\rangle \end{matrix} \quad (16)$$

Downfolding the high energy states leads then (to leading order in  $1/U_d$ ) to

$$H_{\text{eff}} \approx -\frac{2t_{pd}^2}{U_d - \Delta_{pd}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{2t_{pd}^4}{U_d(U_d - \Delta_{pd})^2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \quad (17)$$

The first term is the same energy shift as for parallel spins (15). The additional term is of the same type as that found for the kinetic exchange mechanism. Again, it can be written in terms of spin operators. In the present case they are the spin operators for the  $d$  orbitals, while the  $p$  orbital does no longer appears in the spin Hamiltonian. The spin coupling is now given by

$$J = \frac{4t_{pd}^4}{U_d(U_d - \Delta_{pd})^2}, \quad (18)$$



which reflects that the superexchange mechanism involves four hopping processes (see figure 4), while kinetic exchange only involves two hoppings (see figure 2).

## 2 Hubbard model

We now turn to extended systems with correlations. The simplest model describing itinerant correlated electrons is the Hubbard model [5]

$$H = -t \sum_{\langle ij \rangle \sigma} c_{j\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \quad (19)$$

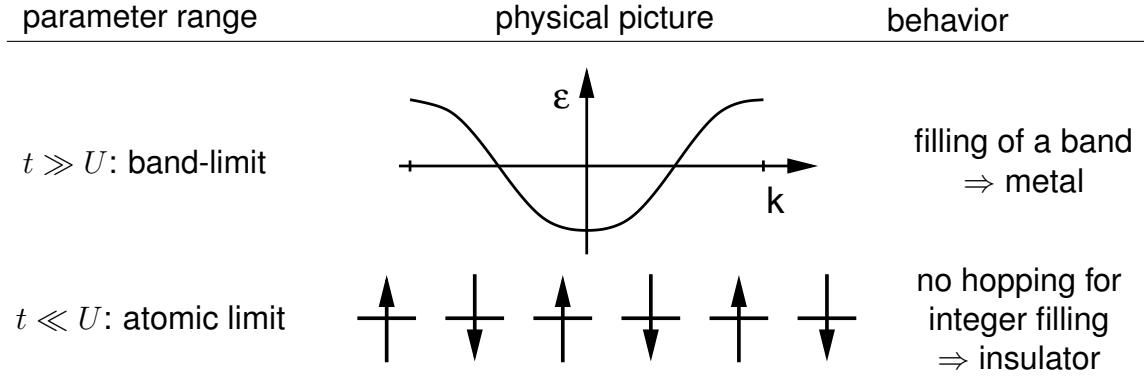
As in our models for the exchange mechanisms, each atom is presumed to have a single relevant orbital with room for two electrons. There are links between the neighboring atoms with matrix elements  $t$ , which can be intuitively interpreted as hopping from site to site. In the absence of other terms the hopping gives rise to a band. A second energy scale is given by the Coulomb repulsion  $U$  between two electrons on the same atom. If this on-site Coulomb repulsion is comparable to or even larger than the band width, the electrons are no longer independent; since the double occupation of an atom is energetically very costly, the movement of an electron will be hindered by the Coulomb repulsion. One says that the electrons move in a *correlated* way. We should note that also the Pauli principle hinders the movement of an electron. This effect can, however, be efficiently described by constructing a Slater determinant from independent-electron wave functions. Correlations, on the other hand, are notoriously difficult to describe since no simple wave functions for such systems are available. In the case of strong correlations, i.e., for  $U \gg t$ , we will treat the hopping as a perturbation. This is called the *atomic limit*, since the sites are almost independent. Thus it is most appropriate to describe strongly correlated electrons in a local picture, i.e. in terms of electron configurations, which are the states that diagonalize the Coulomb term.

### 2.1 Mott transition

The physics described by the Hubbard model is the interplay between kinetic energy and Coulomb repulsion. Writing the Hubbard-Hamiltonian either in real or in  $k$ -space

$$\begin{aligned} H &= -t \sum_{\langle ij \rangle \sigma} c_{j\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ &= \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{U}{M} \sum_{k,k',q} c_{k\uparrow}^\dagger c_{k-q\uparrow} c_{k'\downarrow}^\dagger c_{k'+q\downarrow} , \end{aligned}$$

where  $M$  is the number of lattice sites, we see that there are obviously two limiting cases: There is the non-interacting, or band-limit, when  $t \gg U$ . In that case, only the hopping term survives, i.e., there are no interactions, and the Hamiltonian can be solved easily in  $k$ -space. The energy levels then form a band, and the system is metallic, except when the band is completely filled. In the opposite case, the atomic limit, the interaction term dominates. In that limit, to minimize the Coulomb energy, the electrons will be distributed over the lattice sites as uniformly as possible. For a non-degenerate, half-filled system this means, that every site carries exactly one electron, and hopping is suppressed, because it would create a doubly occupied site, which would increase the energy by  $U \gg t$ . Thus in the atomic limit the half-filled system will be



**Fig. 5:** Metal-insulator transition for half-filling, i.e., one electron per site.

an insulator. Clearly, in-between these two limiting cases there must be, at some value  $U_c$ , the so-called *critical*  $U$ , a transition from a metallic to an insulating state — the Mott transition [6]. Usually this transition is expected when  $U$  becomes of the order of the (non-interacting) band width  $W$ .

As the criterion for determining the metal-insulator transition we can use the opening of the gap for charge carrying single-electron excitations

$$E_g = E(N+1) - 2E(N) + E(N-1), \quad (20)$$

where  $E(N)$  denotes the total energy of a cluster of  $M$  atoms with  $N$  electrons. For the half-filled system we have  $N = M$ . It is instructive to again consider the two limiting cases. In the non-interacting limit the total energy is given by the sum over the eigenvalues of the hopping Hamiltonian  $\sum_{n:\text{occ}} \varepsilon_n$ . Thus, in the non-interacting limit

$$E_g^{\text{band}} = \varepsilon_{N+1} - \varepsilon_N, \quad (21)$$

which, for a partly filled band, will vanish in the limit of infinite system size. On the other hand, in the atomic limit, the Coulomb energy for a single site with  $n$  electrons is  $U n(n-1)/2$ . Thus, for half-filling of we have

$$E_g^{\text{atml}} = U, \quad (22)$$

i.e., the insulating state in the atomic limit is reflected by a finite gap.

For an infinite system the gap  $E_g$  can be rewritten in terms of the chemical potential. In the thermodynamic limit ( $M \rightarrow \infty$  with  $N/M = \text{const.}$ ) we have to distinguish two types: the energy needed to add an electron to the system (electron affinity)

$$\mu^+ = \lim(E(N+1) - E(N)) = \left. \frac{d\varepsilon(n)}{dn} \right|_{n \searrow 1} \quad (23)$$

and the energy required to extract an electron from the system (ionization energy)

$$\mu^- = \lim(E(N) - E(N-1)) = \left. \frac{d\varepsilon(n)}{dn} \right|_{n \nearrow 1} \quad (24)$$

The gap is then given by the discontinuity in the left- and right-derivative of the energy per site  $\varepsilon(n) = \lim E(N)/M$ :

$$E_g = \mu^+ - \mu^-. \quad (25)$$

## 2.2 Heisenberg model

We now consider the Hubbard model in the limit of large  $U$ . This is the generalization of the discussion of kinetic exchange in 1.1 to an extended system. For large  $U$  we work with the electron configurations in which interaction term is diagonal. Configurations with doubly occupied sites will have energies of the order of  $U$  or larger, so these are the configurations that we would like to project out. For downfolding we thus partition the configuration basis, and hence the Hilbert space into the set of low-energy states which have no doubly occupied sites

$$S = \left\{ |n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}, \dots\rangle \mid \forall i : n_{i\uparrow} + n_{i\downarrow} \leq 1 \right\} \quad (26)$$

and the set of high-energy states with one or more doubly occupied sites

$$D = \left\{ |n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}, \dots\rangle \mid \exists i : n_{i\uparrow} + n_{i\downarrow} = 2 \right\} . \quad (27)$$

The hopping term  $T$ , which for large  $U$  is a perturbation to the interaction term  $I$ , couples the subspaces by hopping an electron into or out of a doubly occupied site. In addition it lifts the degeneracies within the subspaces. Hence the Hamiltonian can be partitioned as

$$\hat{H} = \begin{pmatrix} P_S (T + I) P_S & P_S T P_D \\ P_D T P_S & P_D (T + I) P_D \end{pmatrix} , \quad (28)$$

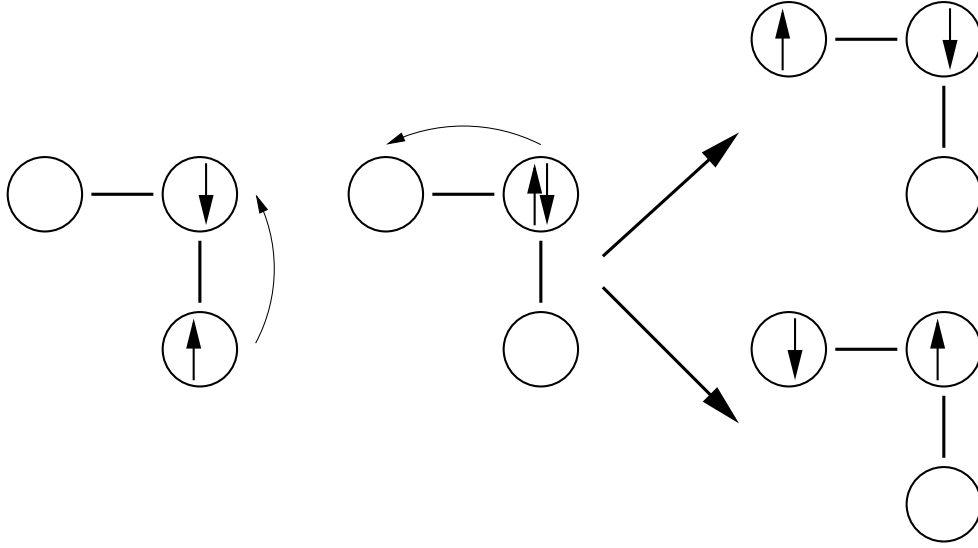
Since we are dealing with an extended system, the subspaces are infinite, so we cannot write the Hamiltonian on the subspaces as matrices. Instead we restrict the operators to the appropriate subspace by using projection operators,  $P_S$  projecting on the low-energy configurations  $S$ ,  $P_D$  projecting on  $D$ . Just like in 1.1 we can then write down an effective Hamiltonian operating on the low-energy configurations only:

$$H_{\text{eff}} = P_S T P_S + P_S T P_D [P_D (\varepsilon - (I + T)) P_D]^{-1} P_D T P_S , \quad (29)$$

Unlike in the derivation of kinetic exchange, for the extended system we have no way of calculating the inverse in the second term explicitly. We can, however, expand in powers of  $t/U$ . This is Kato's method for perturbation theory (see, e.g., sec. 16.3 [7]). Essentially we only need to consider configurations with a *single* double occupancy — these correspond to the states of lowest energy in  $D$ . On this subspace the interaction term is diagonal with eigenvalue  $U$  and can thus be easily inverted. We then obtain the Hamiltonian

$$H_{t-J} = P_S \left[ T - \frac{t^2}{U} \sum_{\langle ij \rangle \langle jk \rangle \sigma \sigma'} c_{k\sigma'}^\dagger c_{j\sigma'} n_{j\uparrow} n_{j\downarrow} c_{j\sigma}^\dagger c_{i\sigma} \right] P_S , \quad (30)$$

which is called the  $t$ - $J$  Hamiltonian. The first term describes the hopping, constrained to configurations with no doubly occupied sites. Thus it essentially describes the hopping of empty sites (holes). To understand what the second term does, we observe that, because of the operators  $n_{j\uparrow} n_{j\downarrow}$ , there are only contributions for states with a singly occupied site  $j$ :  $n_{j\sigma} = 0$  and  $n_{j,-\sigma} = 1$ . After applying the second term, site  $j$  will again be singly occupied with  $n_{j\sigma'} = 0$  and  $n_{j,-\sigma'} = 1$ . Hence, for  $\sigma \neq \sigma'$  the spin on site  $j$  will be flipped. Moreover, we distinguish the contributions where only two different sites are involved ( $k = i$ ) from the three-site terms ( $k \neq i$ ). The terms for  $k = i$  are just the ones we already know from the kinetic exchange



**Fig. 6:** Processes contained in the three-site term  $T'$ : The three-site term describes indirect hopping processes to a second-nearest neighbor site with an intermediate (virtual) doubly occupied state. In the first process the two hopping processes are performed by the same electron, in the second process each electron hops once and thus the spin on the intermediate site is flipped.

mechanism. The three-site terms describe a second-nearest neighbor hopping of an electron from site  $i$  to site  $k$  via a singly occupied intermediate site  $j$ . For  $\sigma = \sigma'$  the spin of the hopping electron is opposite to that on the intermediate site. For  $\sigma \neq \sigma'$  the spin of the intermediate site is flipped — as is that of the hopping electron (see figure 6). The  $t$ - $J$  Hamiltonian can thus be written as

$$H_{t-J} = P_S [T + H_H + T'] P_S \quad (31)$$

with

$$T = -t \sum_{\langle ij \rangle, \sigma} c_{j\sigma}^\dagger c_{i\sigma} \quad (32)$$

$$H_H = \frac{4t^2}{U} \sum_{\langle ij \rangle} \left( \vec{S}_j \cdot \vec{S}_i - \frac{n_i n_j}{4} \right) \quad (33)$$

$$T' = -\frac{t^2}{U} \sum_{\substack{\langle ij \rangle \langle jk \rangle \\ i \neq k}} \sum_{\sigma} \left( c_{k\sigma}^\dagger (1 - n_{j\sigma}) c_{i\sigma} - c_{k,-\sigma}^\dagger c_{j\sigma}^\dagger c_{j,-\sigma} c_{i\sigma} \right) n_{j,-\sigma} \quad (34)$$

In the case of half-filling, when  $n_i = 1$ , all hopping processes are suppressed, i.e. the projection  $P_S$  annihilates  $T$  and  $T'$ . Thus for a Mott insulator the  $t$ - $J$  model reduces to the spin 1/2 Heisenberg model

$$H_H = J \sum_{\langle ij \rangle} \vec{S}_j \cdot \vec{S}_i + \text{const.} \quad (35)$$

with the exchange coupling  $J = 4t^2/U$  given by the kinetic exchange mechanism. We again stress that the spin-spin interaction is a result of projecting out the states with double occupancies.

### 3 Exact Diagonalization

We now discuss how the ground-state of an interacting system can be determined in practice. Considering a Hubbard model

$$H = \sum t_{ij} c_{j\sigma}^\dagger c_{i\sigma} + U \sum n_{i\uparrow} n_{i\downarrow} \quad (36)$$

on a cluster of finite size, the problem is conceptually quite simple: As the system is finite, so is the Hilbert space. Explicit examples we have seen in the first part of the lecture, where we discussed the exchange mechanisms: The Hamiltonian is a finite matrix. This could then be simply diagonalized with standard methods, as discussed, e.g., in the lecture of I. Gutheil. There is, however, a serious *practical* problem: It is true that the Hilbert space is finite, but its dimension grows combinatorially with system size, making it effectively impossible to even store the full Hamiltonian matrix, let alone diagonalize it in a straightforward way. As an illustration, table 1 lists the dimensions of Hilbert spaces of the Hamiltonian (36) for clusters of  $M$  lattice sites and different numbers of electrons:

$$\text{dimension of Hilbert space} = \binom{M}{N_\uparrow} \times \binom{M}{N_\downarrow}. \quad (37)$$

In order to find the ground-state even for systems that are so large that we cannot store the full Hamiltonian, we use a special property of the Hubbard Hamiltonian: hopping is only to near neighbors, and the interaction is local. Therefore the matrix elements of the Hamiltonian are almost all zero. Only between states that differ by the hopping of one electron and on the diagonal, the matrix elements are non-zero. Such a matrix with only a few non-zero entries is called *sparse*. To specify the Hamiltonian we therefore only have to store the non-zero matrix elements. In addition, we can quite efficiently calculate the product of the Hamiltonian matrix with a state-vector,  $H|v\rangle$ . Efficiently here means, that computing time and storage increase “only” linearly with the dimension of the Hilbert space. Nevertheless, since this dimension increases extremely quickly with system size, the method is still confined to relatively small systems.

#### 3.1 Power method and variational minimization

Methods for finding the extremal eigenvalues of a matrix  $H$  work in *Krylov space*, a space generated by repeatedly ( $n$  times) applying  $H$  to some, usually arbitrarily chosen, initial vector  $|v_0\rangle$ . Krylov spaces, spanned by the vectors  $\{|v_0\rangle, H|v_0\rangle, \dots, H^n|v_0\rangle\}$  are useful, because with increasing  $n$  they very quickly have a large overlap with the extremal eigenvectors of  $H$ . To understand why, let us assume we knew the complete eigensystem of  $H$ :  $H|\Psi_k\rangle = \varepsilon_k|\Psi_k\rangle$ . Then we could expand  $|v_0\rangle$  as  $|v_0\rangle = \sum_k c_k |\Psi_k\rangle$ . Applying  $H$  once we thus obtain

$$H|v_0\rangle = \sum_k \varepsilon_k c_k |\Psi_k\rangle, \quad (38)$$

i.e. the eigenvector with the largest  $\varepsilon_k$  is multiplied by the largest number. If we normalize  $H|v_0\rangle$  and again apply  $H$  to the result, the contribution of the largest eigenvector is further enhanced, such that the series of normalized vectors

$$|\tilde{v}_n\rangle = \frac{1}{||H^n|v_0\rangle||} H^n|v_0\rangle \quad (39)$$

M	$N_{\uparrow}$	$N_{\downarrow}$	dim of Hilbert space	memory
2	1	1	4	
4	2	2	36	
6	3	3	400	
8	4	4	4 900	
10	5	5	63 504	
12	6	6	853 776	6 MB
14	7	7	11 778 624	89 MB
16	8	8	165 636 900	1263 MB
18	9	9	2 363 904 400	17 GB
20	10	10	34 134 779 536	254 GB
20	1	1	400	
20	2	2	36 100	
20	3	3	1 299 600	9 MB
20	4	4	23 474 025	179 MB
20	5	5	240 374 016	1833 MB
20	6	6	1 502 337 600	11 GB
20	7	7	6 009 350 400	44 GB
20	8	8	15 868 440 900	118 GB
20	9	9	28 210 561 600	210 GB
20	10	10	34 134 779 536	254 GB

**Table 1:** Dimension of Hilbert space  $\dim(\mathcal{H})$  und computer memory required for storing a single many-body wave-function for Hubbard models with  $M$  orbitals and  $N_{\uparrow} + N_{\downarrow}$  electrons. The first group of numbers gives the dimensions for half-filling, where the Hilbert space is largest. The second group shows how the dimension grows with the filling. Note that the dimensions are symmetric about half-filling. Note also that the fourth column can be interpreted as something like a half-logarithmic plot of the  $\dim(\mathcal{H})$  as a function of system size or filling.

converges to the eigenvector of  $H$  which has the eigenvalue with the largest modulus.

To calculate the lowest eigenstate of  $H$  we again use a Krylov space. We start with some randomly choosen, but normalized initial vector  $|v_0\rangle$  and apply the Hamiltonian to obtain a second vector. These two vectors span a two-dimensional subspace of the Hilbert space, and we can use, e.g., the variational principle to find the lowest energy state on this subspace. To simplify the calculation, we first orthogonalize the vectors, giving

$$|v_1\rangle = H|v_0\rangle - \langle v_0|H|v_0\rangle |v_0\rangle . \quad (40)$$

Should  $|v_1\rangle$  vanish, then  $|v_0\rangle$  already was an exact eigenstate of  $H$ . Otherwise, normalizing, with  $b_1^2 = \langle v_1|v_1\rangle$ , we obtain

$$|\tilde{v}_0\rangle = |v_0\rangle \quad \text{and} \quad |\tilde{v}_1\rangle = \frac{1}{b_1} |v_1\rangle . \quad (41)$$

For this orthonormal basis of the two-dimensional subspace, we name diagonal matrix elements of the Hamiltonian

$$a_0 := \langle \tilde{v}_0 | H | \tilde{v}_0 \rangle \quad \text{and} \quad a_1 := \langle \tilde{v}_1 | H | \tilde{v}_1 \rangle , \quad (42)$$

while the off diagonal matrix element is

$$\langle \tilde{v}_0 | H | \tilde{v}_1 \rangle = \frac{1}{b_1} \langle v_0 | H | v_1 \rangle = \frac{1}{b_1} \langle v_1 | v_1 \rangle = b_1 , \quad (43)$$

where we have used the orthogonality of  $|v_0\rangle$  and  $|v_1\rangle$ . A general, normalized wavefunction in the space spanned by  $|v_0\rangle$  and  $H|v_0\rangle$  is then given by

$$|\Psi\rangle = \cos(\theta)|\tilde{v}_0\rangle + \sin(\theta)|\tilde{v}_1\rangle . \quad (44)$$

Minimizing the expectation value

$$\langle \Psi | H | \Psi \rangle = a_0 \cos^2(\theta) + 2b_1 \sin(\theta) \cos(\theta) + a_1 \sin^2 \theta \quad (45)$$

with respect to the free parameter  $\theta$ , we obtain the quadratic equation

$$b_1 \tan^2(\theta) + (a_1 - a_0) \tan(\theta) - b_1 = 0 \quad (46)$$

where we have divided by  $\cos^2(\theta)$ , i.e., assuming that the randomly chosen state  $|v_0\rangle$  is not already an eigenstate of the full Hamiltonian. Solving for  $\theta$  we find the lowest-energy state on the subspace spanned by  $|v_0\rangle$  and  $H|v_0\rangle$ . Alternatively, we can diagonalize the Hamiltonian matrix

$$H_{|\tilde{v}_0\rangle, |\tilde{v}_1\rangle} = \begin{pmatrix} a_0 & b_1 \\ b_1 & a_1 \end{pmatrix} \quad (47)$$

in the orthonormal basis  $|\tilde{v}_0\rangle$  and  $|\tilde{v}_1\rangle$ .

We can now use the variational lowest-energy state that we found as a new starting vector  $|v_0\rangle$  and start the two-step minimization procedure over again. If we do this repeatedly, we will get a series of vectors with decreasing energy, eventually converging to the ground state. Convergence is guaranteed by the variational principle, except in the case where the initial starting vector happened to be exactly orthogonal to the ground state. In this unlikely case also all subspaces generated by applying the Hamiltonian to this starting vector stay exactly orthogonal to the ground state.

### 3.2 Lanczos method

The Lanczos method [8–11] is the generalization of the above two-step variational minimization technique to larger subspaces. Again, we start from a (randomly chosen) initial vector  $|v_0\rangle$ . From this we generate new states by applying multiplying with the Hamiltonian and orthogonalizing to the previous state in the iteration:

$$|v_1\rangle = H|v_0\rangle - \frac{\langle v_0 | H | v_0 \rangle}{\langle v_0 | v_0 \rangle} |v_0\rangle \quad (48)$$

$$|v_2\rangle = H|v_1\rangle - \frac{\langle v_1 | H | v_1 \rangle}{\langle v_1 | v_1 \rangle} |v_1\rangle - \frac{\langle v_1 | v_1 \rangle}{\langle v_0 | v_0 \rangle} |v_0\rangle , \quad (49)$$

or, more generally

$$|v_{n+1}\rangle = H|v_n\rangle - a_n|v_n\rangle - b_n^2|v_{n-1}\rangle , \quad (50)$$

where

$$a_n = \frac{\langle v_n | H | v_n \rangle}{\langle v_n | v_n \rangle}, \quad b_n^2 = \frac{\langle v_n | v_n \rangle}{\langle v_{n-1} | v_{n-1} \rangle}. \quad (51)$$

Defining  $b_0 = 0$  and  $|v_{-1}\rangle = 0$  this describes the full iteration ( $n = 0, 1, 2, \dots$ ). Normalizing the vectors  $|v_n\rangle$ , i.e., in the orthonormal basis

$$|\tilde{v}_n\rangle = \frac{1}{\sqrt{\langle v_n | v_n \rangle}} |v_n\rangle \quad (52)$$

we obtain, in a similar way as above, the Hamiltonian matrix on the subspace spanned by the vectors  $H^n|v_0\rangle$ :

$$H = \begin{pmatrix} a_0 & b_1 & 0 & 0 & \cdots \\ b_1 & a_1 & b_2 & 0 & \cdots \\ 0 & b_2 & a_2 & b_3 & \cdots \\ 0 & 0 & b_3 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (53)$$

So in the Lanczos iterations (50), we generate a basis, in which the Hamiltonian is tridiagonal. However, for transforming the full Hamiltonian we have to calculate as many matrix-vector products  $H|v\rangle$  as the dimension of the Hilbert space. What makes the Lanczos method so powerful is the fact, that we can stop the iteration after only a few of steps  $N$ . Even if  $N$  is of the order of a few tens — and this number of steps is fairly independent of the actual dimension of the Hilbert space — we find a state that is already extremely close to the ground state [12, 13]. So in practice, we only have to calculate a few products of the Hamilton matrix with a state vector and in the end diagonalize a quite small, tridiagonal matrix. A manageable task, if only we have enough memory to store the vectors that are needed in the iteration (50). Important further applications of essentially the same iteration scheme are to the calculation of spectral functions [8, 9, 11] and the extension to finite temperatures [14, 15].

## Appendices

### A Pauli matrices

Here we collect the most important properties of the Pauli matrices. The Pauli or spin matrices are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (54)$$

They are hermitean, i.e.  $\sigma_i^\dagger = \sigma_i$ , and  $\sigma_i^2 = 1$ . Therefore their eigenvalues are  $\pm 1$ . The eigenvectors of  $\sigma_z$  are  $|m_z\rangle$ ,  $m_z = \pm 1$ :

$$|+1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (55)$$

For these vectors we find

$$\sigma_x|m_z\rangle = |-m_z\rangle \quad \sigma_y|m_z\rangle = im_z|-m_z\rangle \quad \sigma_z|m_z\rangle = m_z|m_z\rangle \quad (56)$$



The products of the Pauli matrices are  $\sigma_x \sigma_y = i\sigma_z$ , where the indices can be permuted cyclically. From this follows for the commutator

$$[\sigma_x, \sigma_y] = 2i\sigma_z \quad (57)$$

while the anticommutator vanishes:

$$\{\sigma_x, \sigma_y\} = 0 \quad (58)$$

Finally a rotation by an angle  $\phi$  about the axis  $\hat{n}$  changes the spin matrices

$$R_{\hat{n}}(\phi) = e^{-i\hat{n} \cdot \vec{\sigma} \phi/2} = \cos(\phi/2) - i \sin(\phi/2) \hat{n} \cdot \vec{\sigma} \quad (59)$$

## B Downfolding

To integrate-out high-energy degrees of freedom, we partition the Hilbert space of the full system into states of interest (low-energy states) and ‘other’ states, which will be integrated out. The Hamiltonian is then written in blocks

$$H = \begin{pmatrix} H_{00} & T_{01} \\ T_{10} & H_{11} \end{pmatrix}, \quad (60)$$

where  $H_{00}$  is the Hamiltonian restricted to the states of interest (reduced Hilbert space),  $H_{11}$  the Hamiltonian for the ‘other’ states, and the  $T$  matrices describe transitions between the two subspaces. The Greens function is partitioned likewise

$$G(\varepsilon) = (\varepsilon - H)^{-1} = \begin{pmatrix} \varepsilon - H_{00} & T_{01} \\ T_{10} & \varepsilon - H_{11} \end{pmatrix}^{-1}. \quad (61)$$

Calculating the inverse of the  $2 \times 2$  matrix, taking into account that the entries are matrices themselves and thus do not commute (see, e.g., *Inversion by Partitioning* in the highly recommended section 2.7 of [16]), we obtain

$$G_{00}(\varepsilon) = (\varepsilon - [H_{00} + T_{01}(\varepsilon - H_{11})^{-1}T_{10}])^{-1}. \quad (62)$$

This expression looks just like the Greens function for a Hamiltonian

$$H_{\text{eff}} = H_{00} + T_{01}(\varepsilon - H_{11})^{-1}T_{10} \quad (63)$$

on the reduced Hilbert space. This effective Hamiltonian describes the physics of the full system, but operates only on the small reduced Hilbert space. Of course, this drastic simplification comes at a price: the effective Hamiltonian is energy dependent. If the hopping matrix elements in  $T_{01}$  are small, and/or if the states in the part of the Hilbert space that has been integrated out are energetically well-separated from the states that are explicitly considered, this energy dependence can to a good approximation be neglected. We can then replace  $\varepsilon$  by a typical energy  $\varepsilon_0$  for the states in the reduced Hilbert space to obtain an energy-independent Hamiltonian  $H_{\text{eff}}(\varepsilon_0)$  that to a good approximation describes the electrons in the reduced Hilbert space, i.e., the states with an energy close to  $\varepsilon_0$ .

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