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Calculation of parameters in model Hamiltonians

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The *ab initio* calculation of parameters of the Anderson model is illustrated within the framework of a simple, exactly solvable, model of a $3d$ compound. It is shown how the latter model can be mapped onto a simpler model, by projecting out degrees of freedom, and by including these degrees of freedom implicitly as a renormalization of parameters. For the model studied this approach is shown to be exact in the limit when the projected degrees of freedom correspond to very delocalized electrons.

I. INTRODUCTION

The local-spin-density (LSD) approximation of the density-functional (DF) formalism[1] has been found to give a rather good description of many weakly or moderately strongly correlated systems.[2] For strongly correlated systems the LSD approximation gives, however, in many situations qualitatively incorrect results. In these situations one could, in principle, introduce a complete one-electron set $|i\rangle$ and calculate the matrix elements of the Hamiltonian. For strongly correlated systems, however, this approach leads to a many-body problem which normally cannot be solved with sufficient accuracy with currently available methods. Alternatively, one can instead introduce a model Hamiltonian, where one keeps the states and interactions believed to be most important for the physics of the problem. Other interactions, which are often not small, are assumed to be included implicitly as a renormalization of the parameters in the model Hamiltonian.

An example is the Anderson-impurity model,[3] where one includes a localized level, a set of extended levels, the hopping matrix elements between these two sets of levels, and the Coulomb interaction between electrons in the localized level. One could try to "derive" the Anderson model from the full Hamiltonian by projecting out the degrees of freedom not included explicitly in the Anderson model. If these degrees of freedom correspond to very delocalized electrons (large hopping integrals), this approach would result in an operator which, to a good approximation, is equal to the Coulomb interaction in the Anderson model, but with a *renormalized* value for the coefficient (Coulomb integral).

Because of the complexity of the full Hamiltonian, such an approach would, however, be extremely complicated for a real system. It would furthermore result in interactions not included explicitly in the Anderson model. These would then have to be transformed away, leading to further renormalizations of the parameters. It is therefore customary to follow a different approach, where the parameters are related to atomic data,[4] calculations in the Hartree-Fock (HF) approximation,[5,6] or in more recent work the LSD approximation.[7-17] In this approach we ask simple questions within the model Hamiltonian framework, directly related to the parameters, and then answer the same question in the LSD approximation for the full system including the degrees of freedom projected out in the model Hamiltonian. For instance, to calculate the position of a localized level or Coulomb integrals, we set the hopping matrix elements equal to zero. In the Anderson model the localized electrons are then decoupled, and they are described by the Hamiltonian

$$H=\varepsilon_{3d}\sum_{m\sigma}n_{m\sigma}+\frac{U}{2}\sum_{(m\sigma)\neq(m'\sigma')}n_{m\sigma}n_{m'\sigma'}\ , \tag{1}$$

where ε_{3d} is the energy of the localized level, U is the Coulomb integral, m is the azimuthal quantum number, and σ is the spin. For this Hamiltonian we can easily find the energy as a function of the occupation number $n=\sum_{(m\sigma)}\langle n_{m\sigma}\rangle$,

$$E(n)=\varepsilon_{3d}+\frac{U}{2}n(n-1)\ . \tag{2}$$

It then immediately follows that

$$\varepsilon_{3d}=E(1)-E(0)\ , \tag{3}$$

$$U=E(2)+E(0)-2E(1)\ . \tag{4}$$

We have left out an uninteresting constant $E(0)$ in Eqs. (1) and (2). We now perform an LSD calculation in which the hopping matrix elements to the localized level have been suppressed. In this way we avoid including these hopping matrix elements implicitly in the calculation of U, since this would lead to double counting. We can also easily specify the occupancy of the localized level and obtain the energy as a function of the occupancy. We can then deduce ε_{3d} and U from the LSD results for the energy differences in Eqs. (3) and (4). In this way the response of the delocalized electrons to a change of the number of localized electrons is included in the calculation of ε_{3d} and U, which are therefore renormalized or "screened" quantities. In some LSD calculations of parameters, the hopping parameters are not set equal to zero. It is then necessary to remove the hopping contribution to the renormalization. This is normally done by performing a mean field calculation for the model Hamiltonian, and then identifying this solution with the LSD results. This approach, however, raises questions about the identification of the mean field and LSD approximations.

The approach described above cannot be justified rigorously for realistic systems, because of the complexity of these systems. It is therefore interesting to study a simple model which can be solved exactly and then apply the approach described above. Within this model we can then see exactly what approximations are introduced in the above-mentioned approach, in what limit these approximations become exact, and how good they are quantitatively in intermediate cases.

In Sec. II we present a simple cluster model of a 3*d* compound. This model is solved analytically in the spinless limit in Sec. III and numerically in the spin-degenerate case in Sec. IV. Some of these issues have been discussed earlier in the context of another exactly solvable model, which includes coupling to plasmons.[18]

II. MODEL

We consider the simple cluster model

$$H=\sum_{\sigma}\left[\sum_{i=1}^{4}\varepsilon_i n_{i\sigma}+(t\psi_{1\sigma}^{\dagger}\psi_{2\sigma}+V\psi_{3\sigma}^{\dagger}\psi_{4\sigma}+\mathrm{H.c.})\right]+U_{dd}n_{2\uparrow}n_{2\downarrow}+U_{ll}\sum_{\sigma\sigma'}n_{1\sigma}n_{3\sigma'}+U_{sd}\sum_{\sigma\sigma'}n_{2\sigma}n_{4\sigma'}\ , \tag{5}$$

which could be seen as a simple example of a 3*d* compound, say NiO. Level 1 represents a ligand orbital (O 2*p* for NiO) and level 2 a 3*d* orbital (Ni 3*d* for NiO), for which we have included the 3*d* Coulomb interaction U_{dd}. These two orbitals are coupled by a hopping integral *t*. The 3*d* orbital interacts with a 4*s* orbital 4 (Ni 4*s*) via the Coulomb interaction U_{sd}, and the 4*s* orbital is coupled via the hopping integral *V* to some other extended orbital 3 (say O 3*s*). Finally, there is a Coulomb interaction U_{ll} between orbitals 1 and 3. These terms are illustrated schematically in Fig. 1. The system has four electrons for the spin-degenerate case and two electrons in the spinless case which will be discussed in Sec. III. Half the electrons are in levels 1 and 2 and the rest in levels 3 and 4. We want to simplify the model to a Hamiltonian where only the 3*d* and ligand level 1 are included, which corresponds to an Anderson model with only one conduction state. We consider, however, the case where the interaction U_{sd} (and perhaps U_{ll}) is so large that it cannot simply be neglected. In Sec. III we will discuss how this can be done analytically for a spinless model of type (5) in the appropriate limit, and in Sec. IV we will numerically perform calculations for the full model with spin.

III. SPINLESS CASE

In this section we study the case when all spins have been suppressed in the model. The aim is to project out states 3 and 4, and to be left with a model containing only states 1 and 2 but with renormalized energies for these levels. We are interested in the case when the hopping *V* between level 3 and level 4 is a very large quantity. The antibonding combination of 3 and 4 is then much higher in energy than the bonding combination. We therefore want to project out the antibonding state, which removes the dynamics of states 3 and 4. This leaves us with the localized level 2 and the extended state 1, which corresponds to the Anderson model in the limit when the conduction band is replaced by one single level. Within the framework of our simple model, this corresponds to the mapping of the real system onto the Anderson model (the Anderson model with one conduction state).

We perform this mapping in a way which is rather closely related to the LSD calculation of parameters. We introduce bonding an antibonding solutions for the system $\{|3\rangle,|4\rangle\}$ in the presence of an electron in level 1 or level 2, respectively. With an electron in level 1 we have the solutions

$$\psi_{b1}=a_3\psi_3+a_4\psi_4\ , \tag{6}$$

$$\psi_{a1}=a_4\psi_3-a_3\psi_4\ . \tag{7}$$

With an electron in level 2 we instead have the solutions

$$\psi_{b2}=\tilde{a}_3\psi_3+\tilde{a}_4\psi_4\equiv(\cos\phi)\psi_{b1}+(\sin\phi)\psi_{a1}\ , \tag{8}$$

$$\psi_{a2}=\tilde{a}_4\psi_3-\tilde{a}_3\psi_4\equiv(\cos\phi)\psi_{a1}-(\sin\phi)\psi_{b1}\ , \tag{9}$$

where $\sin\phi$ is of the order $1/V$. We have used the notations $\cos\phi$ and $\sin\phi$ to indicate that, e.g., ψ_{b1} and ψ_{b2} are rather similar. The states Eqs. (6)–(9) have the energies ε_{b1}, ε_{a1}, ε_{b2}, and ε_{a2}, respectively. In an LSD type of calculation we would obtain the energies ε_{b1} and ε_{b2} and introduce effective level positions for the reduced two-level problem,

$$\varepsilon_1^{\mathrm{eff}}=\varepsilon_1+\varepsilon_{b1}\ , \tag{10}$$

$$\varepsilon_2^{\mathrm{eff}}=\varepsilon_2+\varepsilon_{b2}\ . \tag{11}$$

The effective hopping matrix element is in such an approach assumed to be the unrenormalized parameter *t*.

To obtain the exact solution of the model (5), we define a complete basis set of orthogonal many-electrons states

$$|\tilde{1}\rangle=\psi_1^{\dagger}\psi_{b1}^{\dagger}|0\rangle\ , \tag{12}$$

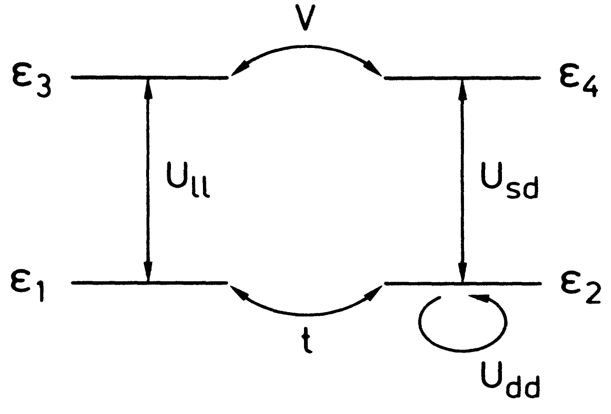

FIG. 1. Schematic illustration of the levels in model (5).

$$|\tilde{2}\rangle=\psi_2^\dagger\psi_{b2}^\dagger|0\rangle\ , \tag{13}$$

$$|\tilde{3}\rangle=\psi_1^\dagger\psi_{a1}^\dagger|0\rangle\ , \tag{14}$$

$$|\tilde{4}\rangle=\psi_2^\dagger\psi_{a2}^\dagger|0\rangle\ . \tag{15}$$

This leads to the resolvent operator

$$(z-H)^{-1}=\begin{bmatrix} z-\varepsilon_1-\varepsilon_{b1} & -t\cos\phi & 0 & t\sin\phi \\ -t\cos\phi & z-\varepsilon_2-\varepsilon_{b2} & -t\sin\phi & 0 \\ 0 & -t\sin\phi & z-\varepsilon_1-\varepsilon_{a1} & -t\cos\phi \\ t\sin\phi & 0 & -t\cos\phi & z-\varepsilon_2-\varepsilon_{a2} \end{bmatrix}^{-1} . \tag{16}$$

The poles of this operator determine the exact eigenvalues and eigenvectors of the problem.

We not focus on the upper left 2×2 corner of (16), which corresponds to the two-level problem involving levels 1 and 2. We can now fold the lower right corner into the upper left corner, using a projection operator (Löwdin folding[19]) technique. The elements in the upper left corner are then replaced by more complicated operators, and we have to study the 2×2 matrix

$$(z-\tilde{H})^{-1}\ . \tag{17}$$

For instance, the 11 element takes the form

$$\tilde{H}_{11}=\varepsilon_1+\varepsilon_{b1} + \frac{t^2\sin^2\phi(z-\varepsilon_1-\varepsilon_{a1})}{(z-\varepsilon_1-\varepsilon_{a1})(z-\varepsilon_2-\varepsilon_{a2})-t^2\cos^2\phi}\ . \tag{18}$$

Equation (17) still gives exact eigenvalues, and we have mapped the 4×4 problem onto a 2×2 problem exactly. The price we have to pay for this reduction is, however, that the quantities $\tilde{H}$ are in general energy dependent. We now focus on the low-lying states, assuming that V is larger than the other energies in the problem. For the two low-lying states we then have

$$z-\varepsilon_1-\varepsilon_{a1}\approx z-\varepsilon_2-\varepsilon_{a2}\approx 2V\ . \tag{19}$$

To second order in $1/V$ we can then set

$$\tilde{H}_{11}=\varepsilon_1+\varepsilon_{b1}\ , \tag{20}$$

where the correction terms are of the type $\sim(U_{sd}-U_{ll})^2t^2/V^3$. The diagonal elements of the reduced problem are then identical to the results for the effective level positions determined above [Eqs. (10 and (11)]. These levels have *first*-order corrections in $1/V$, due to the screening by levels 3 and 4 projected out of the problem. In addition, the hopping matrix element $t\cos\phi$ has a *second*-order renormalization, normally neglected in the determination of hopping parameters. The renormalization is simply the overlap between the bonding solutions $|b1\rangle$ and $|b2\rangle$, when an electron is in level 1 or 2, respectively.

The above approximation is analogous to the adiabatic approximation for an electron-nuclear system. We assume that the electrons in the system $\{|3\rangle,|4\rangle\}$ can follow the electrons in the system $\{|1\rangle,|2\rangle\}$ perfectly. This is true to leading order in $1/V$, while to higher order there are "nonadiabatic" effects leading to excitations into the antibonding level, and a corresponding reduction of the hopping to the bonding level. Such effects are neglected in the determination of effective parameters. This approach therefore relies on the assumption that the system has two quite different types of electrons, one set of localized electrons and another set of electrons which can effectively follow the motion of the electrons in the first set.

IV. SPIN-DEGENERATE CASE

In the spin-degenerate case we have to consider a 16×16 matrix to obtain the exact solution. This is complicated to treat analytically, and we rely on a numerical solution. In Table I we show exact results for the ground-state energy E_0, the occupancy n_{3d} of level 2, and the susceptibility

$$\chi=-\partial^2E_0(H)/\partial H^2\ .$$

In the calculation of χ we assume a coupling $-H(n_{2\uparrow}-n_{2\downarrow})$ to the magnetic field H.

We furthermore calculate renormalized parameters in the same spirit as has been done for realistic systems and as was already done for the spinless case. Thus we set $t=0$ and calculate the ground-state energy $E(n_2)$ as a function of the occupancy n_2 of the localized level 2. The values of $\varepsilon_2^{\text{eff}}$ and U_{dd}^{eff} are deduced from Eqs. (3) and (4). We then solve the spin-degenerate two-level problem with these renormalized parameters. The results are shown in Table I under the column headed "Renormalized." As expected from the discussion in Sec. III, the agreement between the approximate and exact results is very good when V is larger than all other energies in the problem. However, even for V as small as 1 the approximate results are surprisingly good.

For large values of V the readjustment of the electrons in the space $\{|3\rangle,|4\rangle\}$ to the electrons in the space $\{|1\rangle,|2\rangle\}$ is very small, since the energy cost of such an adjustment is very large compared with the reduction in the interaction energy due to the Coulomb interaction

TABLE I. The ground-state energy E_0, the occupancy n_{3d} of the $3d$ level, and the susceptibility $\chi = -\partial^2 E_0(H)/\partial H^2$ of the spin-degenerate model (5). We have used the parameters $\varepsilon_1=\varepsilon_2=\varepsilon_3=\varepsilon_4=0$, $t=1$, $U_{dd}=4$, $U_{sd}=2$, and $U_{ll}=0$.

V	$\varepsilon_2^{\text{eff}}$	U^{eff}	E_0 Renormalized	E_0 Exact	n_{3d} Renormalized	n_{3d} Exact	χ Renormalized	χ Exact
1.0	1.17	3.18	−3.05	−2.95	0.380	0.364	0.314	0.312
1.5	1.39	3.21	−3.97	−3.90	0.339	0.326	0.266	0.262
2.0	1.53	3.29	−4.92	−4.88	0.317	0.307	0.240	0.237
3.0	1.68	3.44	−6.87	−6.85	0.292	0.287	0.214	0.213
4.0	1.75	3.55	−8.85	−8.84	0.280	0.277	0.202	0.201
6.0	1.83	3.68	−12.83	−12.82	0.268	0.267	0.190	0.190
10.0	1.90	3.80	−20.81	−20.81	0.259	0.258	0.181	0.181
20.0	1.95	3.90	−40.80	−40.80	0.252	0.252	0.174	0.174

U_{sd}. Therefore U^{eff} is close to its unrenormalized value $U=4$, and $\varepsilon_2^{\text{eff}}$ is close to the value $U_{sd}\langle n_4\rangle$, where $\langle n_4\rangle$ is the occupancy of level 4. As V is reduced the adjustments in the space $\{|3\rangle,|4\rangle\}$ are larger, and the energy cost for adding one or two electrons to the "$3d$ level" (level 2) is lower. Thus the values of $\varepsilon_2^{\text{eff}}$ and U^{eff} are reduced.

The photoemission spectrum was obtained by calculating the final states with one electron less than the ground state, and by taking matrix elements between these states and the ground state of an electron annihilation operator. The results are shown in Table II. The two-level model gives a quite accurate description of the two lowest peaks for $V=10$. For $V=2$ the description is, as expected, less accurate, in particular for the weak second peak. In all cases the two-level model entirely misses a number of very weak peaks at larger energies. These peaks correspond to degrees of freedom suppressed in the two-level model. In the two-level model we have assumed that the electrons in the states projected out can adjust perfectly to any change in the localized electrons. In reality, there is a certain probability that this adjustment does not take place. The system then ends up in a final state with a higher energy, which is reflected in the high-lying low-weight satellites. As V increases, and the mobility of the electrons projected out of the problem increases, the weight of these satellites is reduced. If we nevertheless are interested in these satellites, we clearly have to use the full four-level model.

V. DISCUSSION

We have studies a simple model of a transition metal compound. By projecting out degrees of freedom, we obtained a model similar to the Anderson model, but with more complicated operators. These operators can be replaced by the normal operators describing the level positions and Coulomb interaction, if the suppressed degrees of freedom correspond to very delocalized electrons. The coefficients of these operators are, however, renormalized by the degrees of freedom projected out. In our example the renormalization is of the order $1/V$, where V is the hopping matrix element between the levels projected out of the problem. We demonstrated how these renormalized parameters can be obtained by studying the response of the delocalized electrons to changes in the number of localized electrons. This is an analogy to the approach used for calculating the parameters of real system using the LSD approximation.

In our calculation in Sec. III, the hopping matrix t has a second-order renormalization in $1/V$, i.e., the renormalization is of higher order than for the level positions. The situation need not, however, remain this simple for more complicated models. An example is a model where the localized level expands spatially when its occupancy

TABLE II. The photoemission spectrum from level 2 ("$3d$"). Results are shown for $\varepsilon_1=\varepsilon_2=\varepsilon_3=\varepsilon_4=0$, $U_{dd}=4$, $U_{sd}=2$, $U_{ll}=0$, $t=1$, and $V=2$ and $V=10$. Results are shown for the peak positions and peak weights according to the exact calculation and according to the two-level model with renormalized parameters.

$V=2$				$V=10$			
Energy		Weight		Energy		Weight	
Renormalized	Exact	Renormalized	Exact	Renormalized	Exact	Renormalized	Exact
0.4259	0.4095	0.1526	0.1418	0.3799	0.3787	0.1256	0.1248
2.9428	2.7995	0.0057	0.0026	3.1387	3.1338	0.0038	0.0037
	4.5801		0.0087		20.3957		0.00049
	7.1616		0.00004		23.2170		0.00001
	8.6287		0.00017		40.4083		0.0000006
	11.6849		0.000001		43.3046		0.00000001

is increased.[20] This greatly increases the hopping matrix elements, and it is an example of how the Coulomb interaction between the localized electrons can renormalize the hopping matrix elements. In general, this effect cannot, however, be completely described just as a renormalization of the parameters in the Anderson model, but it requires a slight generalization of the model by introducing hopping matrix elements which depend on the occupancy of the localized level.[20] The renormalization of the hopping matrix elements due to the Coulomb interaction between localized and delocalized electrons has also been discussed.[21] In this case it is found that there is an energy-dependent renormalization, which is particularly efficient for thermodynamic properties.

It is relatively easy to study the renormalization resulting from the suppression of degrees of freedom in simple models of the type discussed here. For a model giving a realistic description of a real system, this approach, however, becomes very complicated. In addition, this approach in general leaves us with interactions not included in the model we want to obtain. To take these interactions into account by a further renormalization of the parameters is not straightforward. It is therefore often difficult to tell exactly what renormalizations should be included, in particular for the hopping matrix elements. Apart from the configuration dependence already mentioned, it has therefore normally been assumed that there are no renormalization effects for the hopping parameters, beyond what has been included implicitly through the LSD exchange-correlation potential. It is for the moment not very clear to what extent this is justified. Most calculations[7,9,12,14] of hopping parameters suggest that this approach is reasonable, although few attempts have been made to estimate the errors involved. In calculations for Ce compounds, it has, however, been found that this approach overestimates the hopping matrix elements.[15] Whether this overestimate is due to the LSD approximation or the neglect of renormalization effects is, however, not known.

When using a simple model Hamiltonian of the type already discussed, we single out "important" Coulomb interactions between "localized" levels and keep these interactions in the model. We observe that even if the basis set is complete, this approach is not invariant under unitary transformations among the basis functions. To obtain meaningful results, we therefore need a sensible definition of the localized orbital. This is a less serious problem if the localized orbital really is very localized, as in the case of the $4f$ orbital in Ce compounds or the $3d$ orbital in many transition element compounds, since the calculated value of the Coulomb integral should then be relatively insensitive to the precise definition of the localized orbital. On the other hand, in La_2CuO_4 it is found that about 30% of the oxygen $2p$ orbital is located outside the oxygen Wigner-Seitz sphere. In a case like this the definition of the proper localized orbital is much more ambigous.

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