WHAT UNDERLIES THE ANDERSON HAMILTONIAN?*

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CONF-860789--3

DE87 004991

October 1986

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To be published in the proceedings from the International Workshop on Condensed Matter Theories, July 21-26, 1986, Argonne National Laboratory.

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*This work supported by the U.S. Department of Energy, BES-Materials Sciences, under Contract W-31-109-ENG-38.

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ABSTRACT

The Anderson Hamiltonian characterizes a model in which local orbitals interact with each other through Coulomb interactions and with a bath of itinerant states through hybridization. It has been utilized with considerable success to discuss phenomena ranging from the Kondo problem to the occurrence of two peaks in the photoemission spectra of Ce compounds. Normally, it is studied by examining the content of its solutions. Of comparable significance, however, is the determination of the various parameters entering the model. In trying to find a prescription for the parameters of the model, one simultaneously develops some understanding of the states involved and studies whether the model incorporates enough of the essential physics. One useful tactic is to compare this model with other models and ask how different effects are accommodated. Here, I will compare results from the model with atomic, band, and modified band calculations for f-electron materials. In light of the complexity of the problems posed, it should be appreciated that I will concentrate more on posing questions than on providing answers.

My interest in the actual content of the Anderson Hamiltonian [1] was kindled by its utilization to interpret the photoemission spectra of Ce compounds. Beyond my natural disinclination to accept claims that this (or any) model was the answer, I was quite concerned that it did not appear to incorporate effects that seemed to be significant. Specifically, it is difficult to see the relation of this model to the multiple-screening-mode model [2,3] which is a natural interpretation of our band calculations. Yet the Anderson model can represent the experimental situation reasonably well. One could always casually dismiss its success by saying that it is mere curve fitting, with model parameters that have been assigned phenomenologically [4]. But that would be a bit too cavalier in light of the added fact that f-counts derived from it correlate at least qualitatively with those found in band calculations. Thus arises the question of just what can be

*Work supported by the U. S. Department of Energy, BES-Materials Sciences, under contract #W-31-109-ENG-38.

represented in a model Hamiltonian of the Anderson form. Such an examination needs to be done very carefully if it is to be useful. Consider a different example: that of the spin Hamiltonian. If one has not been properly introduced to it, one would naturally assume that the spin Hamiltonian is nothing more than a phenomenological model. Yet it can be related to utilization of the spin-coordinates to describe what is occurring in the associated underlying spatial wave function. (Normal usage is, of course, as a phenomenological model.) Let us examine the Anderson Hamiltonian in a similar fashion. To do this, we first represent the computations as a surrogate for the experiment and then consider how this model Hamiltonian might represent the effects observed. A proviso is in order: it is not so much my intent to present solutions as to pose questions.

Selected Density Functional Theory

Density functional theory is based on the observation that the ground state properties (and the total energy in particular) are functionals of the density ($E=E[\rho]$). There is, of course, the problem that one does not know these functionals and they must be approximated, but when the intra-atomic repulsion U is truly the dominant factor, this will not be critical. This direct Coulomb interaction (which is explicitly included) will far overshadow any uncertainty in our knowledge of the exchange-correlation functionals. Writing the density as a sum of single particle amplitudes,

$$\rho = \sum \psi_k^* \psi_k$$

the ψ_k must satisfy single-particle-like equations of the form

$$(t + V) \psi_k = e_k \psi_k.$$

Here, t is a single-particle kinetic-energy operator and V incorporates the self-consistent Hartree field plus the functional derivative of the exchange-correlation functional (usually evaluated in the local density approximation -- but that is not of concern here). The total energy is not a simple sum of the eigenvalues e_k but must include the effects of Coulomb double counting and the involved functional form of the exchange correlation functional. The eigenvalue e_k is a functional of all the other occupied orbitals and will reflect changes occurring in those orbitals. A particularly useful observation that will be exploited extensively is the relation [5]

$$e_k = dE/dn_k,$$

which states that the eigenvalue is the local derivative of the energy. (This energy is the analytic continuation of the total energy, which is strictly valid only at integral occupation values rather than the more physical energy of a statistical ensemble. Consequently, questions of discontinuous behaviour do not enter this discussion.) To study the photoemission process, we must break slightly with the formal theory, which limits itself to the ground state or to ensembles of states. Making that leap of faith, we nonetheless will be accounting for the major Coulomb interactions, including those that are responsible both for screening and for the intra-atomic repulsion U . As the occupation number n_k is changed, the eigenvalue e_k will change to reflect the changes occurring in the entire (model) many-body system. In essence, this theory is mapping the energetics of a many-body system onto a set of one-particle eigenvalues. A natural consequence is that as one excites the system, these eigenvalues will change! If the excitation is spatially delocalized, the change will be negligible.

When it is not, one can integrate on the occupation number from one down to zero to obtain the removal energy. However, as the eigenvalue is very nearly a linear function of the occupation number, one of several simple things can be done: one can calculate at the half integral value (which is the standard transition state prescription) or, as will be useful here, one can use the average of the eigenvalues obtained with the orbital fully occupied and completely empty.

An Atomic Case Study

To make this a bit more concrete, consider the results of a series calculations on cerium and uranium atoms involving transitions between f- and d-orbitals. The total energy can be written

$$E_T = e_f^0 n_f + U_f n_f^2/2 + e_d^0 n_d + U_d n_d^2/2 + X_{df} n_d n_f + E_o(n_d, n_f),$$

where E_o represents the response of the s electrons and the core to changes in the d and f occupation. With the assumption that this dependency can also be adequately expanded to quadratic order, we may redefine the parameters appearing in the remainder of the expression to include these additional terms (relaxation effects) and treat E_{oo} as constant. The eigenvalues are then the derivative of this expression (I -- as well as many others -- have checked that this is really so [6]):

$$e_f = e_f^0 + U_f n_f + X_{df} n_d$$

$$e_d = e_d^0 + U_d n_d + X_{df} n_f$$

For the uranium atom, we can make the approximation $U_d \sim 0$ and consider $(f^3 d^2 s^1) \rightarrow (f^{2.5} d^{2.5} s^1)$ to find $U_f = 3.4$ eV and $X_{df} = 0.7$ eV. This leaves about 1-1.5 eV for solid state screening. With the tripositive ion, one finds $U_f \sim 25.6$ eV and $X_{df} \sim 7.3$ eV more nearly akin to the unscreened result. In the case of cerium, we do not make the $U_d \sim 0$ approximation and we find $U_f \sim 12$ eV, $U_d \sim 6$ eV, and $X_{df} \sim 7$ eV. These parameterizations represent the behaviour of the eigenvalues reasonably well. Note now that if we fix $n_d = 1$ and look at the dependence of e_f on n_f ,

$$e_f(1) = e_f^0 + U_f + X_{df},$$

$$e_f(0) = e_f^0 + X_{df},$$

and the removal energy is

$$\Delta_f = e_f^0 + U_f/2 + X_{df}.$$

Because $U_f > 0$, Δ_f will appear at greater binding energy than the eigenvalue $e_f(1)$. Again, such careful consideration is required for local orbitals as a price for mapping many-body behaviour onto a set of single-particle-like quantities. The band supercell calculations [7-9] to be discussed presently indicate that, for the Ce compounds, an f to d transition is more appropriate:

$$\Delta_{fd} = e_f^0 - e_d^0 - U_f/2 - 3U_d/2 + X_{df},$$

which differs from the ground state eigenvalue difference by

$$\delta_{\text{relax.}} = U_f/2 - U_d/2 + X_{df}$$

for $(f^1 d^1 s^2) \rightarrow (f^0 d^2 s^2)$. This is actually not the best case because this is a very large energy. It is reduced when the atom is compressed into a solid and the s state is converted to a d state. Nonetheless, it does demonstrate the difficulty of reaching the f^0 state -- which is a crucial point in mixed-valence discussions.

Multiple Screening Mode Model in a Solid

To discuss photoemission from the f-states on a Ce atom in a solid, the model we have applied is based on the following assertions:

1. Transitions from the f-orbitals are local excitations -- no matter whether the ground state wave function is or is not local. This requires that we deal with a special excited (i.e., impurity) atom. This is done by forming a supercell consisting of the excited atom surrounding "host" atoms, repeated as a periodic array.
2. The Total Energy difference must be determined to find the excitation energy. This is, after all, a many-body problem. Although there are some formal fine points to worry about in what we do, we at least include the major direct Coulomb interactions -- including the U term of the Anderson Hamiltonian! We usually -- but not always -- utilize eigenvalue arguments like the ones used above to get at this total energy difference.
3. The transitions occur into channels which are the different possible screening states -- i.e., excited states of the many-body problem. These must be postulated. Those that we consider are as follows:
 - a. A fully (f-) screened peak which will occur very near the eigenvalue in the ground state potential because the potential is changed very little as a consequence of the similarity between the screening charge and the charge of the removed electron. (We believe the ESCA-type transitions and band f- transitions to be very improbable.) Because the ground state eigenvalues occur at or very near the Fermi energy, these transitions will occur very near but not necessarily exactly there as well. The fact that the screening arises from the remaining f-orbitals can provide an explanation of the observation of the spin-orbit splitting in that peak [10].
 - b. A poorly screened state which is created by forcing an f-hole and then letting the system relax. The hole is screened by a Ce d-electron and the binding energy appears about 2.5 eV below the fully screened peak.
 - c. An "unscreened" peak (perhaps seen in CeN) which could appear 5-7.5 eV below the fully screened peak. This energy is obtained in the renormalized atom calculation [11] (as the eigenvalue), partly as a consequence of the use of Hartree-Fock formalism in the renormalized atom calculations and partly as a consequence of the local unhybridized form assumed for the f-orbital.

Several results are obtained from this model. The peak separation between the fully and the partially screened peak agrees very well with those observed for Ce materials; this finding gives some credibility to the results. The poorly screened peak appears to be very well described as a d-screened f-hole. One thus sees approximately an atomic transition, which explains the fact that the peak separation is roughly constant (it does increase slightly as one proceeds down the iso-electronic pnictide series). The f-eigenvalues calculated in the f^0 state are very flat bands, indicating that the hybridization has been

"turned off" in that state. The one exception in the series is CeN, where the strong admixture into the nitrogen p-bands indicates that the state is actually unstable. This is experimentally manifested by the absence of a second peak in CeN. Apparently, a similar situation occurs in the uranium materials. One important additional observation needs to be made concerning the ground state alone: the f-density always consists of two spin-orbit split atomic-like levels just above the Fermi energy, with a tail, pulled below that energy by the hybridization, containing roughly one f-electron for the cerium materials and roughly 2.5 electrons for the uranium materials. This is a result of the calculation -- not an input -- and will need to be rationalized with the Anderson model parameter E_f .

Relation to Anderson Model

Now let us examine how these features might appear in the Anderson model. Anderson [1] originally proposed this model Hamiltonian to study local moment formation of transition metal impurities in metals. The essence of the problem, which this rather schematic model is intended to capture twofold is: (1) The almost core-like d- or f-orbitals are strongly correlated (H_{corr}) by their strong intra-atomic Coulomb repulsion -- with the small radial extent greatly enhancing the size of $\langle 1/|r_1 - r_2| \rangle$. (2) Because these orbitals are not for a free atom in a vacuum, they must couple with the surrounding sea of electrons (H_{cf}). The model is better tuned to the Kondo problem than the photoemission problem because the former does not involve a net change in the number of local orbitals. The form of the Hamiltonian is

$$H = H_c + H_f + H_{\text{cf}} + H_{\text{corr}}.$$

H_c represents an unperturbed conduction electron sea:

$$H_c = \sum_K \epsilon_K n_{K\sigma}.$$

Because the focus is on the local orbitals, this sea of conduction electrons is viewed as a rather structureless bath which can be treated as nearly free electrons -- Anderson suggested Orthogonalized Plane Waves (OPWs). H_f represents our "free" local orbitals which, although they were d-orbitals for Anderson, will now be our f-orbitals:

$$H_f = E_f (n_+ + n_-).$$

The form for a single orbital with spin degeneracy is used for notational simplicity. The generalization to the degenerate case is normally utilized, but only f^0 , f^1 , and f^2 are taken as significant in the treatment of Ce materials (and the comparable hole states for Yb). As a consequence, it is reasonable to avoid introducing the additional exchange parameters in H_{corr} below. The presence of spin-orbit coupling, producing an $f_{5/2} - f_{7/2}$ splitting, is actually the more important consideration complicating the selection of lowest-lying levels. It is to be noted here that, from the form of the Hamiltonian, E_f is the change in total energy as the number of f-electrons is changed from zero to one if there is no hybridization. This will be significant in the comparisons to be made below. H_{cf} is the single-particle-like hybridization term:

$$H_{\text{cf}} = \sum (V_{\text{kf}} c_{k\sigma}^* c_{f\sigma} + \text{Hermitian conj.}).$$

V_{kf} embodies the Coulomb and exchange interactions between the local orbital and the member of the conduction electron sea. The correlation term is

$$H_{\text{corr}} = K(n_+ + n_-)(n_+ + n_-)/2 - J(n_+n_+ + n_-n_-)/2 \sim Un_+n_-.$$

It is the size of U that provides the first and most dramatic hint that one needs to consider the precise nature of the underlying structure represented by this model. If one simply uses atomic or ionic wave functions to estimate U , one arrives at values two to ten times larger than those derived from the analysis of experiment.

Clearly, this Hamiltonian is for an impurity problem, which is a reasonable model for the photoemission process involving the f -orbital since the excited atom becomes an impurity in the lattice. Because this is an impurity model, it is reasonable to make a unitary transformation on the conduction sea from Bloch (i.e., k) states to site-centered levels. With this mapping, one focuses more on $\rho(e)$ than on the $e_{k\sigma}$ themselves. This expediency of mapping k into $\{e, n\}$ has been utilized by Gunnarsson and Schoenhamer [4] in their extensive analysis of the model. To actually carry it through in practice is a rather more subtle problem because, as in the problem of Wannier functions, there is the matter of the optimal choice of phases [12].

The form of this model assumes the underlying states to be orthogonal. One might think that in light of the core-like nature of the $4f$ orbital, this would not be difficult to arrange. However, the conduction electrons do have $\ell=3$ character that penetrates at least as far as the tail region of the $4f$ -orbital. One can realize this either by observing that a plane wave will have $\ell=3$ character associated with a spherical Bessel function or by considering the Lowdin α -expansion of the orbitals from the neighboring atoms about the Ce site. Is this non-orthogonality not likely to be the source of the concept of two types of f -electrons? Anderson clearly thought so in the case of the d -states [1]. Orthogonality can always be arranged by a suitable transformation of states. It has long been known that orthogonalization weakens the hybridization interaction. So practitioners of the combined interpolation schemes [13] perform the orthogonalization step first and only then set up the hybridization term. Within the Anderson model, this property is the basis for Zitzkova and Rivier's observation that non-orthogonality effects narrowed the resonance [14]. This transformation to an orthogonal basis set is also the origin of the direct $k \rightarrow k'$ scattering which they observe and is also mentioned by Harrison [15]. The majority of the non-orthogonality effects can be absorbed into a simple redefinition of the parameters. Only this scattering is not so accommodated -- at least in the Bloch representation -- but I suspect that it could be similarly incorporated as merely a renormalized $\rho(e)$ and $V(e)$ in the site-specific representation. One way to explore this idea is to perform the extraction of this information from the non-orthogonal Slater-Koster band parameterization rather than the orthogonal version used for YbP [16].

It is a stringent approximation that the conduction electrons states are taken to be the same independent of the condition of the local orbitals. If the set of states is sufficiently complete, the response can be described by changes in occupation alone. But perhaps a better description is achieved by considering the modifications of the states produced in response to changes in local (i.e., f -) orbital occupation at the site. This can be illustrated by considering Anderson's suggestion that one use OPWs. Because the $4f$ orbital is roughly the same size as the $4d$ and $5s, 5p$ orbitals in Ce, these orbitals will be rather strongly interacting. These core orbitals will be changed according to whether the $4f$ is occupied or not. If these orbitals are changed, then certainly the OPWs will be changed as well. Although this effect has not been incorporated in models of valence

electron spectroscopies, it has for the core electron spectroscopies [17-19]. It is precisely the significance of this effect which is at issue in the discussions of the interpretation of L_{III} absorption. And it enters as well in the comparison of the Anderson model with the multiple-screening-mode interpretation for the two-peak structure.

It is the omission of the direct Coulomb interactions involving the conduction electron sea (and the core electrons) that gives the Anderson model its simplicity. But these effects must then be absorbed in the remaining terms. Is it possible? This is the crucial question because this interaction is the driving term for screening and as such is needed to relate the Anderson mode to the multiple-screening-mode model [2-3]. The band structure results [7-9] indicate that the major screening process is generally the population of an additional d-like orbital. Forming a d-screened f-hole excitation may well be the key to transforming away the direct Coulomb interaction, but this would definitely modify all the parameters. To illustrate, returning to the atomic case, one could write n_d as a linear function of n_f (expanding about $n_f=1$ for Ce) and rewrite E_T and Δ_{fd} as a function of n_f alone. To do this for the solid, one must assume that the atom never makes a transition to a different charged state: the fully screened f^1 and the partially (i.e., d-) screened f^0 state both have the same charge. But what of the f^2 state? That would appear to be properly described as well, because an anti-screening occurs when an extra f-electron is added [20]. This type of approach would accommodate the fact that in the atom it costs less energy to add an extra f-electron than an extra d-electron. Such an approach would allow one to appropriately incorporate the core relaxations as well. The remaining screening effects on the f-orbitals might well be incorporated by defining the appropriate "medium" of s- and p-electrons. This scheme has the nice feature that it incorporates the relative stability of the peak separation by tying it to an f to d transition which is only slightly modified by the solid state environment.

Now, however, what is the effect on the hybridization term of the Hamiltonian? Note that the redefined f^0 state can scatter the conduction electron and will also require additional effort to maintain the orthogonalization. Is it possible to transform these effects such that they appear in the $\rho(e)$? Even if one ends up with modifications of the $V(e)$ and $\rho(e)$, this would not result in dramatic changes because the photoemission does not appear to depend critically on this structure. However, there is the problem that the explanation used for the non-existence of a second peak in CeN is the strong coupling of the f^1 state to the conduction bands when the system is in the f^0 state. How could this effect appear in the modified model? The best way to proceed at this point is to attempt to further refine the definitions suggested above, get the problem into a second quantized form rather than the qualitative c-number discussion given, and then attempt a transformation to the form of the Anderson Hamiltonian -- probably with the introduction of a few averages along the way. This is a necessary program to understand the application of an Anderson-like model for the Ce compounds.

It is interesting to note that the situation is somewhat different in the Yb compounds. In the Yb materials, one must transform to a hole language, but one then has the complementary problem, except that now the f-orbitals are much more localized owing to the lanthanide contraction. The consequence is that the hybridization is weaker and the model is more directly applicable. There may be core relaxation effects but not the d-orbital screening. This would be consistent with the idea that the heavy lanthanides are less tolerant of d-states than

the lighter lanthanides [21]. The effect is due to the much smaller size of the cores in the heavier lanthanides. This can best be illustrated by some recent computer experiments. We set up the f-orbitals as core states such that we could control the f-count. The band states were forced to be orthogonal to the f-states by only including variational freedom for the 5f states. Calculations were then done for two assumed configurations, f^{13} and f^{14} (each is a sort of supercell consisting entirely of impurity atoms). When the conduction states were examined, very nearly rigid-band behaviour was found, in which the densities of states for the two calculations were almost identical between the two Fermi energies found, and corresponded to the one additional electron. The implication is that the Anderson model is more easily applied to the Yb compounds. That is why we have begun studies on the Yb systems first [16] rather than on the Ce compounds.

Two general observations should be made. (1) It was noted earlier that the principal peaks of the f-character always appear above the Fermi energy in the band calculations for Ce compounds. This is an immediate consequence of applying Fermi statistics. Yet the Anderson model is only interesting if E_f is below the Fermi energy. This apparent discrepancy is resolved if one notes that E_f is the change in total energy occurring when the f-count is decreased or increased by one in the absence of hybridization. Thus E_f is more nearly to Δ_{fd} in the case of Ce and Δ_f in the case of Yb ($f^{13} \rightarrow f^{14}$). These terms include relaxation and screening effects. The band eigenvalue position is merely a local derivative and not a representative of what happens when the occupation changes by one. Thus E_f is not placed by these peaks in the f density of states but is displaced by an amount demonstrated above for the atomic case. (2) In the Anderson model, the hybridization mixes the two spin states [1]. A similar feature appears in the band calculations for the $j=5/2$ and $j=7/2$ states. In a strongly hybridized material, the two spin-orbit split peaks in the density of states will occur well above the Fermi energy with long tails extending down into the occupied states. There will be a large component of $f_{7/2}$ character. As the hybridization becomes weaker, the $f_{5/2}$ derived peak will fall to the Fermi energy, which then occurs in the leading edge of that peak, and the $f_{7/2}$ component will not be occupied. Consequently, the fractional $f_{7/2}$ occupation is a good index of the strength of hybridization.

This discussion really ends with questions rather than conclusions. Suggestions have been made for relating the Anderson model to the multiple-screening-mode model. In the process of doing so, the difficulties in defining the parameters of the model to make them amenable to calculation become apparent. Nonetheless, one would like to try to make that connection, since it would more clearly define the mechanisms acting in these "highly correlated" materials. The problem appears more tractable in the case of the Yb materials than the Ce materials. In the Yb materials, one can work with something close to "bare" particles, whereas in the Ce materials one is committed to defining a set of quasi-particles such as a d-screened f hole, for example. If one succeeds in doing so, will one be able to justify using the same entities for the low-energy (i.e., low-temperature) properties? Given that hybridization and the intra-atomic interaction of the local orbitals are the major significant concepts, it is at least as important to explore how one might be able to transform the entire many-body problem to such a simplified form that a more detailed solution could be sought. But the screening of a charge is also an important concept in this problem. Utilizing a multiple-screening-mode model, one can rationalize a very large body of systematics for core excitations [22]. Unfortunately, charge screening is also a difficult problem not

well represented by a linear theory. It would be nice if one were able to schematize it in some way such as folding its effects into the parameters of the Anderson model. Further research in this area would be most significant and useful, and might well lead to breakthroughs in the understanding of mixed-valent and heavy Fermion systems.

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