THE DERIVATION OF EFFECTIVE HAMILTONIANS

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It is discussed how to obtain, from a single pair of equations, the effective hamiltonians commonly used in solid state physics as well as their corresponding perturbative expansions.

The widespread use of effective hamiltonians makes it desirable to develop a simple and general method for their derivation. Van Vleck [1] seems to have been the first to show how to transform a given hamiltonian in order to obtain, in a perturbative fashion, an effective hamiltonian representing the effect of the original hamiltonian on the manifold of eigenvectors of a certain chosen unperturbed eigenvalue. Kato [2,3] made afterwards a rigorous analysis of the mathematical structure and convergence of operator perturbation theory. Matrix techniques have been used for the same problem by Löwdin [4] for the first orders of perturbation theory. Almost thirty years had to go by since the original work of Van Vleck until Bloch [5] gave an explicit equation for a projected transformation operator generating an effective hamiltonian for a single manifold. Later des Cloizeaux [6] and the present author [7] independently showed how to modify the projected transformation operator introduced by Bloch in order to obtain projected effective hamiltonians which are hermitian to all orders of perturbation theory. In between, Primas [8,9] had presented an elegant way of obtaining at once an effective hamiltonian H_{eff} for all manifolds of interest. Finally Jørgensen [10], as a remarkable feat, established the connections between the until then apparently unrelated approaches. Unfortunately his careful analysis is encumbered by the fact that he restricts himself to the projections on a single manifold, and this prevents him from finding the relationships between his too many operators.

In what follows it is discussed how to generate all common effective hamiltonians through a simple formalism inspired by the ideas put forward by Primas [8] and Jørgensen [10].

According to current usage an effective hamiltonian associated both with a given hamiltonian H and a soluble part H_0 of H is an operator H_{eff} such that:

(a) it has the same eigenvalues as H,

(b) its eigenvectors are in a one-to-one correspondence with the eigenvectors of H,

(c) it has no matrix elements connecting eigenvectors belonging to different eigenvalues of H_0.

It should be noticed that many of the effective hamiltonians currently used are not hermitian [2,3,5,10] and therefore no restriction is placed in this respect.

Condition (a) means that if

$$H|\Psi\rangle = E|\Psi\rangle , \qquad (1)$$

then

$$H_{\mathrm{eff}}|\Psi\rangle_0 = E|\Psi\rangle_0 . \qquad (2)$$

It should be stressed here that because of condition (c) the eigenvalue problem of H_{eff} may be solved separately for each manifold of degenerate eigenvectors of H_0. The eigenvectors $|\Psi\rangle_0$ are the so-called bonnes fonctions or good zeroth-order eigenvectors, and are not necessarily orthogonal.

Condition (b) implies that there is a non-singular

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transformation operator S such that

$$|\Psi\rangle = S|\Psi\rangle_0\,, \quad |\Psi\rangle_0 = S^{-1}|\Psi\rangle\,. \tag{3}$$

From eqs. (1) to (3) it follows that H_{eff} and H are related by the similarity transformation

$$H_{\mathrm{eff}} = S^{-1}HS\,. \tag{4}$$

Next H is explicitly separated into the soluble part H_0, which is usually suggested by the nature of the problem, and a remainder V,

$$H = H_0 + V\,. \tag{5}$$

The operator V does not necessarily have to be small unless one wishes to take a perturbative approach. This is not always the case because quite frequently one generates effective hamiltonians with disposable parameters to be determined from experiment as in the case of the spin hamiltonians used in the theory of magnetism. It is now convenient to write

$$H_{\mathrm{eff}} = H_0 + W\,, \tag{6}$$

where W is the level-shift operator.

In order to make use of condition (c) we define the projection operator P_j over the manifold of eigenvalue ϵ_j. Therefore

$$H_0 = \sum_j \epsilon_j P_j\,, \tag{7}$$

where by definition $\epsilon_j \neq \epsilon_k$ if $j \neq k$. Defining the diagonal part $\langle A\rangle$ of an operator A with respect to H_0 by [8]

$$\langle A\rangle = \sum_j P_j A P_j\,, \tag{8}$$

condition (c) may now be written

$$H_{\mathrm{eff}} = \langle H_{\mathrm{eff}}\rangle\,, \tag{9}$$

that is,

$$W = \langle W\rangle\,. \tag{10}$$

Upon multiplication of eq. (6) by the left with S, and taking into account eqs. (4) and (5) one obtains

$$[H_0, S] = SW - VS\,. \tag{11}$$

Eq. (11) may now be solved for the non-diagonal part $S - \langle S\rangle$ of the transformation operator giving [8]

$$S = \langle S\rangle + h_0(SW - VS)\,, \tag{12}$$

where h_0 is the superoperator defined by

$$h_0(A) = \sum_{j\neq k}\sum P_j A P_k/(\epsilon_j - \epsilon_k)\,, \tag{13}$$

and $\langle S\rangle$ is an arbitrary diagonal operator.

Taking the diagonal part of eq. (11) and using eqs. (7) and (10) it is found that

$$\langle [H_0, S]\rangle = 0\,, \tag{14}$$

and therefore

$$\langle S\rangle W = \langle VS\rangle\,. \tag{15}$$

From eqs. (12) and (15) it is seen that S is not determined unless its diagonal part $\langle S\rangle$ is given first. We will only require $\langle S\rangle$ to have an inverse. Defining a new operator R by

$$R = S\langle S\rangle^{-1}\,, \tag{16}$$

and using eqs. (12) and (15) it is found that

$$R = 1 + h_0(R\langle VR\rangle - VR)\,, \tag{17}$$

$$W = \langle S\rangle^{-1}\langle VR\rangle\langle S\rangle\,. \tag{18}$$

Therefore R may be solved from eq. (17), and then W is obtained through R and $\langle S\rangle$, the only effect of the latter being to scramble the matrix elements of $\langle VR\rangle$ through the similarity transformation eq. (18).

All usual effective hamiltonians are obtained by making an implicit or explicit choice for $\langle S\rangle$, and by taking different projections of S, S^{-1}, $\langle S\rangle$, $\langle S\rangle^{-1}$, W or its products. Primas [8] chooses, for instance,

$$\langle \ln S\rangle = 0\,. \tag{19}$$

A convenient restriction is to make the similarity transformation eq. (4) a canonical transformation, that is taking S to be a unitary operator,

$$S^{\dagger} = S^{-1}\,. \tag{20}$$

Van Vleck [1] and Primas [8] chose the condition eq. (20).

All schemes of perturbation theory follow from solving eq. (17) through repeated replacements of the second member into the argument of h_0 (for a simple illustration of such a scheme which does not make use of operators, see ref. [11]). The differences come about upon giving the explicit dependence of R on the parameter λ which characterizes the order of smallness of V or of the different contributions to V. It is easy to see that writing H_{eff} to order λ^n is equivalent to saying that one has eliminated the non-diagonal part of V [in the sense of eq. (8)] to that order. In the context of perturbation theory it should also be pointed out that the problem of quasi-degeneracies should never arise because it should always be possible to choose H_0 in such a way that the unperturbed levels ϵ_j are well enough separated, thus providing a fast convergence of the perturbation series.

A sore point in all non-unitary schemes is that the existence of S does not immediately follow and one is not even sure if $|\Psi\rangle_0$ is a non-zero vector. In the unitary version eq. (20) the existence of S follows from the argument that eq. (4) then corresponds to a rotation of H such as to bring its mutually perpendicular principal axes to fall within the mutually orthogonal manifolds ϵ_j. An extrapolation of the two and three dimensional cases indicates that such a rotation should always be possible.

A full discussion of the explicit connections between the different ways of setting up effective hamiltonians and the corresponding restrictions placed on $\langle S\rangle$ and/or S exceeds the space available here and will be made in a later paper.

Summing up, it has been found that all usual methods of generating effective hamiltonians for the case of a discrete spectrum and their corresponding perturbation series are variations and expansions of eqs. (17) and (18).

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