DIAGRAMMATIC ANALYSIS OF ADIABATIC AND TIME-INDEPENDENT PERTURBATION THEORY FOR DEGENERATE ENERGY LEVELS

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Time-ordered folded diagrams are used to represent the effective hamiltonian in the adiabatic formalism. Resummation of the diagrams is shown to give a term-by-term correspondence with time-independent perturbation theory.

1. Introduction

Perturbation theory for a degenerate energy level can be formulated in two essentially different ways. In fact, expressions for the effective hamiltonian are derived both from the familiar time-independent approach and by means of time-dependent adiabatic techniques. In this letter the connection between these two formulations will be investigated. To that end it will be shown how the time-dependent formalism naturally leads to a representation for the effective hamiltonian in terms of time-ordered folded diagrams. Topologically equivalent diagrams have been introduced recently by Kvasnička [1] along different lines; in his formulation the diagrams are not interpreted as being time-ordered. The diagrammatic expansion of the effective hamiltonian will subsequently be resummed in such a way that a term-by-term correspondence is established with the time-independent Rayleigh–Schrödinger theory in the formulation given by Bloch [2].

We shall study the energy-eigenvalue problem for a time-independent hamiltonian $H = H_0 + H_1$, with H_1 a perturbation term. The perturbed eigenvalue problem associated with a degenerate energy level in the discrete spectrum of H_0 can be written in terms of an effective hamiltonian $\mathcal{H} = P_0 \mathcal{H} P_0$, where P_0 is the projector onto the degenerate eigenstates. In the time-dependent interaction representation this effective hamiltonian is given by [3,4]:

$$\mathcal{H} = \lim_{\epsilon\to 0} P_0 H_1 U_\epsilon(0,-\infty) P_0 [P_0 U_\epsilon(0,-\infty) P_0]^{-1} . \quad (1)$$

Here $U_\epsilon(0,-\infty)$ is the adiabatic evolution operator; it is given as a power series in the interaction operator

$$H_{1\epsilon}(t) = \mathrm{e}^{-\epsilon|t|} \mathrm{e}^{\mathrm{i}H_0 t} H_1 \, \mathrm{e}^{-\mathrm{i}H_0 t} \quad (2)$$

by means of the Dyson expansion:

$$U_\epsilon(0,-\infty) = \sum_{m=0}^{\infty} (-\mathrm{i})^m \int_{-\infty}^{0} \mathrm{d}t_1 \ldots \mathrm{d}t_m \, \theta(-t_1) H_{1\epsilon}(t_1) \times \theta(t_1 - t_2) \ldots \theta(t_{m-1} - t_m) H_{1\epsilon}(t_m) . \quad (3)$$

The denominator of (1) can be eliminated by the following way. Each function $\theta(t)$ is split up in $\Theta(t)$ and P_0, with $\Theta(t) \equiv \theta(t)(1 - P_0) - \theta(-t) P_0$. Then the numerator of (1) can in $(m+1)$th order be written as a sum of terms in which the first intermediate P_0 occurs after k operators $\Theta(t)$. Upon choosing k and $m-k$ as the independent summation variables one finds that the numerator of (1) factorizes such that the part involving the sum over $m-k$ exactly cancels the denominator. As a result one gets:

$$\mathcal{H} = \lim_{\epsilon\to 0} \sum_{n=1}^{\infty} (-\mathrm{i})^{n-1} \int_{-\infty}^{0} \mathrm{d}t_1 \ldots \mathrm{d}t_{n-1} P_0 H_{1\epsilon}(0) \Theta(-t_1) \times H_{1\epsilon}(t_1) \Theta(t_1 - t_2) \ldots \Theta(t_{n-2} - t_{n-1}) H_{1\epsilon}(t_{n-1}) P_0 , \quad (4)$$

with $n = k + 1$ denoting the order in the perturbation expansion.

2. Diagrammatic representation of the effective hamiltonian

Formula (4) is our starting point for the diagrammatic representation of the effective hamiltonian. In fact, when the definition of $\Theta(t)$ is substituted the nth order contribution to $\mathcal{H}$ becomes a sum of 2^{n-2} terms that are specified by a unique succession of operators P_0 and $Q_0 \equiv 1 - P_0$. We shall represent these terms by drawing the time variables t_k as vertices, connected by a string of oriented line segments. A downward or upward line segment $(k, k+1)$ corresponds to a projector Q_0 or P_0 between the interaction hamiltonians $H_1(t_k)$ and $H_1(t_{k+1})$; definition of $\Theta(t)$ then implies that in the diagram the upward direction corresponds to increasing time. As an example a sixth-order term from (4), with Q_0, Q_0, P_0, P_0, Q_0 as the successive intermediate projectors, is drawn in fig. 1. Associated with these projectors is the time ordering $0 > t_1 > t_2, t_4 > t_3 > t_2$ and $0 > t_4 > t_5$. However, the order of the vertices is not determined completely by these conditions: the term under consideration actually leads to a set of 11 different diagrams, of which the one with $0 > t_1 > t_4 > t_3 > t_2 > t_5$ is shown in fig. 1.

The contribution to $\mathcal{H}$ from a single diagram is obtained by performing the time integrations. As can be seen from (2) each vertex entails a factor $\exp[i(E_{k-1,k} - E_{k,k+1} - i\epsilon)t_k]$ in the integrand; here $E_{k,k+1}$ is the energy difference between the intermediate state associated with the line segment $(k, k+1)$ and the initial state. Upon integrating over the time variables from the lowest vertex onwards a product of energy denominators results. The real part of the denominators can be read off from the diagram by cutting it horizontally above each of the vertices and adding up, for every intersection, the energies E of the encountered downward lines. The latter are different from zero so that the real parts of all denominators are nonvanishing; the imaginary parts are linear in ϵ and may hence be neglected; in particular this means that the contribution of each separate diagram is finite in the adiabatic limit. Finally we note that every diagram carries a sign $(-1)^q$, with q the number of projectors Q_0. For the diagram of fig. 1 the above prescriptions lead to the product of energy denominators $E_{01}E_{12}(E_{12} + E_{45})^2E_{45}$ and a negative sign.

In this section we have derived rules for a diagrammatic representation of the general term in the effective hamiltonian $\mathcal{H}$. The diagrams came about as a natural consequence of the time-dependent approach for the perturbation theory. Diagrams of the same topological structure have been written down by Kvasnička [1], who obtained them in lowest orders of the perturbation expansion by employing a time-independent formalism. This author already noticed as a general feature the similarity with the folded diagrams of many-body theory. Indeed the latter diagrams may be found from a similar splitting of θ-functions [3,5] as that leading to our eq. (4).

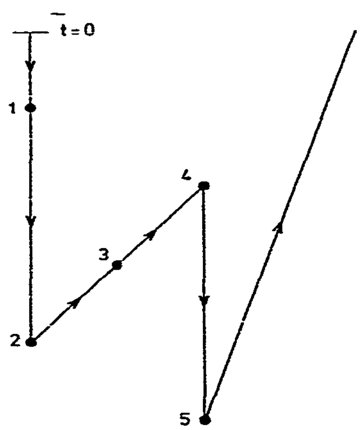

Fig. 1. Folded-diagram representation of a sixth-order contribution to the effective hamiltonian.

3. Connection with time-independent perturbation theory

The effective hamiltonian $\mathcal{H}$ as calculated according to the rules of the preceding section contains energy denominators in which sums of excitation energies E show up. Ordinary time-independent Rayleigh–Schrödinger perturbation theory, however, leads to an expression for $\mathcal{H}$ with products of only single excitation energies in the denominators. Such an expression can indeed be derived from the present formalism.

We study a diagram D of nth order (see fig. 2a) and calculate the $(n-1)$-fold time integral $\mathcal{I}(D)$ over the functions $\theta(t_k - t_{k'})$ and $\exp[i(E_{k-1,k} - E_{k,k+1})t_k]$. Let j be the lowest index such that $t_{j\pm 1} < t_j$ (i.e. t_j is the first relative maximum in the diagram). We shall

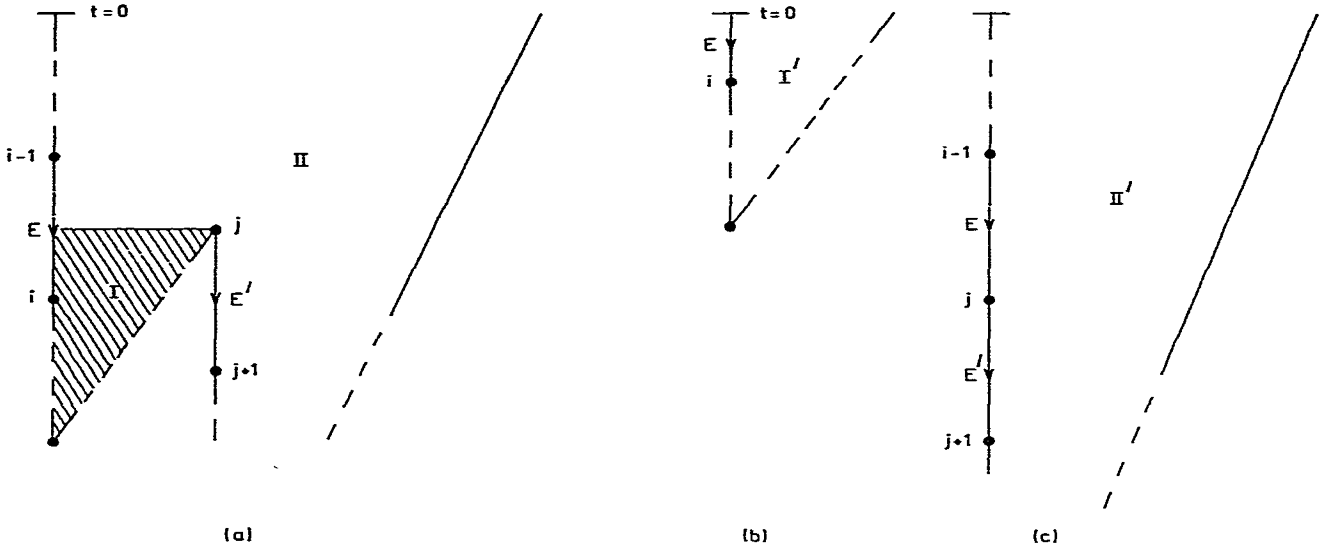

Fig. 2. Factorization of a general diagram $D = D_I + D_{II}$ into a V-type diagram $D_{I'}$ and a remaining diagram $D_{II'}$.

split the diagram into two parts, D_I and D_{II}: D_I contains the lines and vertices up to the point j that have $t < t_j$, and D_{II} is its complement. For each particular diagram D there exist a whole class {D} of diagrams having the same D_I and D_{II}, but a different relative ordering of the vertices in D_I with respect to those in D_{II}. If all diagrams in this class are taken together the integrations over the time variables in D_I, with upper boundary t_j, can effectively be carried out independently from those in D_{II}.

In addition to D_I one may consider a diagram $D_{I'}$ of the same structure in which the integrations run to $t = 0$ (see fig. 2b). In accordance with time-translation invariance the associated integrals are related by $\mathcal{I}(D_I) = \mathcal{I}(D_{I'})\exp(iEt_j)$, with $E = E_{i-1,i}$. In the integrand of $\mathcal{I}(D)$ the vertex j contributes a phase factor $\exp(-iE't_j)$, with $E' = E_{j,j+1}$, so that the total factor containing t_j is $\exp[i(E-E')t_j]$. With this modified phase factor the integrand depending on the time variables of D_{II} (i.e. on $t_1, \dots t_{i-1}, t_j, \dots t_{n-1}$) precisely equals that of the diagram $D_{II'}$, drawn in fig. 2c. As a result we find:

$$\sum_{\{D\}} \mathcal{I}(D) = \mathcal{I}(D_{I'})\,\mathcal{I}(D_{II'})\,. \tag{5}$$

This relation is in fact the analogue of the factorization theorem commonly used in many-body perturbation theory [6].

The argument leading to (5) may be applied iteratively to $D_{II'}$. As a consequence the effective hamiltonian can be rewritten as a sum of "factorized" diagrams D_f that are products of simple V-type diagrams like $D_{I'}$. Since the time integrals $\mathcal{I}$ of the V-diagrams contain no sums of excitation energies in the denominators the same holds true for the diagrams D_f.

The above factorization scheme may be illustrated by means of the diagram in fig. 1, to which two diagrams of the same topological structure must be added, with $0 > t_1 > t_4 > t_3 > t_5 > t_2$ and $0 > t_1 > t_4 > t_5 > t_3 > t_2$, respectively. When the contributions of the three diagrams are summed one arrives indeed at the factorized denominator $E_{01}E_{12}^3E_{45}$.

The general factorized denominator of a diagram D_f is:

$$E_{01}^{k_1}E_{12}^{k_2}\dots E_{n-2,n-1}^{k_{n-1}}\,, \tag{6}$$

with $k_i \geqslant 0$. The exponents $\{k_i\}$ can be read off from D_f. To that end one first has to decompose the diagram into its constituent V-type diagrams in the way indicated before. For the latter the exponents follow straightforwardly from the time integrations. Taking as an example the same sixth-order contribution as before we get a factorized diagram with exponents

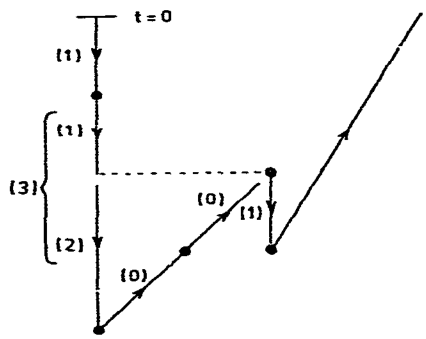

Fig. 3. Factorized sixth-order diagram with exponents (1,3,0,0,1).

(1,3,0,0,1) (see fig. 3); it is built up from two V-diagrams for which the k-values are (2,0) and (1,1,1), respectively.

In a generalized factorized diagram the assignment of the k-values is such that the conditions

$$\sum_{i=1}^{n-1} k_i = n-1, \qquad \sum_{i=1}^{p} k_i \geqslant p, \qquad \forall p < n-1 \tag{7}$$

are satisfied; in fact these constraints are valid already in each of the elementary V-diagrams. Conversely, for a given set of values $\{k_i\}$ fulfilling (7) one constructs in a unique way a diagram D_f.

All diagrams contributing in a factorized diagram D_f are accompanied by the same string of successive projectors P_0, Q_0 and the same overall sign $(-1)^q$, with q the number of projectors Q_0. The energy factors E^{-k} can accordingly be replaced by operators S_k, with $S_0 \equiv P_0$ and $S_k \equiv -Q_0(H_0 - E_0)^{-k}$ for $k > 0$ (E_0 being the unperturbed energy). Thus we have found that each D_f in the diagrammatic expansion of the effective hamiltonian corresponds to an algebraic term

$$P_0 H_1 S_{k_1} H_1 S_{k_2} \ldots S_{k_{n-1}} H_1 P_0 \,. \tag{8}$$

The complete $\mathcal{H}$ is found by drawing all distinct factorized diagrams D_f. This corresponds to a summation of (8) over the exponents $\{k_i\}$, subject to condition (7), and over the order n; the expression thus obtained for the effective hamiltonian was first derived by Bloch [2] in the framework of time-independent perturbation theory. So a term-by-term correspondence has been established between the time-dependent and time-independent formulations of perturbation theory for degenerate energy levels.

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References

[1] V. Kvasnička, Chem. Phys. Letters 32 (1975) 167.
[2] C. Bloch, Nucl. Phys. 6 (1958) 329.
[3] T. Morita, Progr. Theoret. Phys. 29 (1963) 351.
[4] L.N. Bulaevskii, Soviet Phys. JETP 24 (1967) 154.
[5] G. Oberlechner, F. Owono-N'-Guema and J. Richert, Nuovo Cimento 68B (1970) 23;
T.T.S. Kuo, S.Y. Lee and K.F. Ratcliff, Nucl. Phys. A176 (1971) 65.
[6] L.M. Frantz and R.L. Mills, Nucl. Phys. 15 (1960) 16;
H.A. Bethe, B.H. Brandow and A.G. Petschek, Phys. Rev. 129 (1963) 225.