

Normalization of states in perturbation theories

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Simple expressions are given for the normalization coefficients in Rayleigh–Schroedinger, Brillouin–Wigner, and Bloch–Horowitz perturbation methods. These expressions are derivatives of the energy, or of the matrix elements of the effective Hamiltonian.

The problem of the normalization of the perturbed states is often ignored in the discussions on perturbation theory. Since this normalization is needed in the calculation of transition matrix elements, we feel that it is useful to show how to obtain it in a simple way.

The Hamiltonian is divided (as usual) into two terms

$$H = H_0 + h, \quad (1)$$

such that the eigenfunctions and eigenvalues of the first term H_0 (the unperturbed Hamiltonian) are known:

$$H_0|a\rangle = \epsilon_a|a\rangle. \quad (2)$$

We have to solve the Schroedinger equation,

$$H|\Psi\rangle = E|\Psi\rangle. \quad (3)$$

In the limit $h \rightarrow 0$,

$$|\Psi\rangle \rightarrow |0\rangle, \quad E \rightarrow \epsilon_0, \quad (4)$$

and we assume for simplicity that there is no other state with unperturbed energy ϵ_0 .

We briefly review the two usual perturbation treatments, i.e., the Rayleigh–Schroedinger and the Brillouin–Wigner expansions.

Let us start with the Rayleigh–Schroedinger treatment. We denote by E_n and $|\Psi_n\rangle$ the n th order terms in the energy and wave function, respectively,

$$E = \sum_{n=0} E_n, \quad (5a)$$

$$|\Psi\rangle = \sum_{n=0} |\Psi_n\rangle. \quad (5b)$$

If we use the subsidiary condition

$$\langle 0|\Psi_n\rangle = \delta_{n0}, \quad (6)$$

the Schroedinger equation (3) yields¹

$$E_0 = \epsilon_0, \quad |\Psi_0\rangle = |0\rangle,$$

$$E_n = \langle 0|h|\Psi_{n-1}\rangle, \quad |\Psi_n\rangle = \sum_i y_i^{(n)}|i\rangle, \quad (n \geq 1)$$

$$y_i^{(n)} = [1/(\epsilon_0 - \epsilon_i)] \langle i|[(h - E_1)|\Psi_{n-1}\rangle - E_2|\Psi_{n-2}\rangle - \dots - E_{n-1}|\Psi_1\rangle], \quad (7)$$

where $|i\rangle, |j\rangle, \dots \neq |0\rangle$ denote unperturbed states different from the initial one.

The function (5b) is obviously not normalized to unity. Since $|0\rangle$ enters with unit weight in (5b), the amplitude x_0 of the unperturbed state $|0\rangle$ in the perturbed (normalized) wave function is precisely the normalized coefficient that we are looking for. The modulus to the square of this amplitude may be obtained as follows.

In matrix form, Eq. (3) reads

$$\sum_a \langle b|H|a\rangle x_a = E x_b \quad (8)$$

or

$$E = \sum_{a,b} x_b^* x_a \langle b|H|a\rangle. \quad (9)$$

Changing only the matrix elements of H_0 , it follows that

$$|x_0|^2 = \frac{dE}{d\epsilon_0} = 1 - \sum_i \frac{dE}{d\epsilon_i}. \quad (10)$$

Therefore, the normalization coefficient $|x_0|^2$ is obtained through simple derivation of the expression for the energy. This is given in perturbation theory as a sum of products of factors, each factor being proportional to

$$\sum_{i,j,\dots,k} \frac{h_{0i} h_{ij} \dots h_{k0}}{(\epsilon_0 - \epsilon_i)^{\sigma_i} (\epsilon_0 - \epsilon_j)^{\sigma_j} \dots (\epsilon_0 - \epsilon_k)^{\sigma_k}}, \quad (11)$$

where

$$h_{ij} = \langle i|h|j\rangle$$

and σ_n are integer numbers.

We obtain an expression similar to (10) for the Brillouin–Wigner perturbation expansion.² We write the Schroedinger equation to matrix form

$$\begin{pmatrix} H_0 + h & h_{0i} \\ h_{i0} & H_0 + h' \end{pmatrix} \begin{pmatrix} x_0 \\ x_i \end{pmatrix} = E \begin{pmatrix} x_0 \\ x_i \end{pmatrix}. \quad (12)$$

Here h' denotes the part of h that has matrix elements between the states $|i\rangle, |j\rangle, \dots$. Using (12), we obtain the ratio between the amplitudes x_i and x_0 :

$$x_i/x_0 = y_i,$$

$$y_i = - \sum_j \langle i| \frac{1}{H_0 + h' - E} |j\rangle h_{j0}. \quad (13)$$

The well-known equation for the energy follows from (12) and (13)

$$E = W(E)$$

$$\begin{aligned} W(E) &= \epsilon_0 + h_{00} - \sum_{i,j} h_{0i} \langle i| \frac{1}{H_0 + h' - E} |j\rangle h_{j0} \\ &= \epsilon_0 + \sum_{n=1} \sum_{i,j,\dots,k} \frac{h_{0i} h_{ij} \dots h_{k0}}{(E - \epsilon_i)(E - \epsilon_j) \dots (E - \epsilon_k)}, \end{aligned} \quad (14)$$

where n again indicates the order of perturbation.

The eigenvalues of the energy are given by the interaction of the curve $W(E)$ (which in general has poles at the unperturbed energies ϵ_i) with the straight line given by the left-hand side of the first Eq. (14).

The normalization condition for the state $|\Psi\rangle$ is

$$\begin{aligned}
1 &= |x_0|^2 + \sum_i |x_i|^2 \\
&= |x_0|^2 \left(1 + \sum_{i,j,k} h_{0i} \langle i | \frac{1}{H_0 + h' - E} | j \rangle \langle j | \frac{1}{H_0 + h' - E} | k \rangle h_{k0} \right) \\
&= |x_0|^2 \left[1 + \sum_{n=2} \sum_{i,j,\dots,k}^{(n)} \frac{h_{0i} h_{ij} \dots h_{k0}}{(\epsilon_i - E)(\epsilon_j - E) \dots (\epsilon_k - E)} \left(\frac{1}{(\epsilon_i - E)} + \frac{1}{(\epsilon_j - E)} + \dots + \frac{1}{(\epsilon_k - E)} \right) \right]. \quad (15)
\end{aligned}$$

Thus,

$$|x_0|^2 = \left(1 + \sum_i \frac{\partial W(E)}{\partial \epsilon_i} \right)^{-1} = \left(1 - \frac{\partial W(E)}{\partial E} \right)^{-1}. \quad (16)$$

In any point different than an eigenvalue Eq. (14) does not hold. Thus, the derivatives $\partial W(E)/\partial E$ are different from one.

The relation between (10) and (16) is easily established as follows

The derivative of the energy E with respect to ϵ_i is

$$\frac{dE}{d\epsilon_i} = \frac{\partial W}{\partial \epsilon_i} + \frac{\partial W}{\partial E} \frac{dE}{d\epsilon_i} = \frac{\partial W}{\partial \epsilon_i} - \left(\sum_j \frac{\partial W}{\partial \epsilon_j} \right) \frac{dE}{d\epsilon_i}. \quad (17)$$

From (17) we obtain

$$1 = \left(1 - \sum_i \frac{dE}{d\epsilon_i} \right) \left(1 + \sum_i \frac{\partial W}{\partial \epsilon_i} \right), \quad (18)$$

and thus (10) follows from (16) using (18).

The transition matrix elements are given:

$$\begin{aligned}
\langle \Psi_2 | T | \Psi_1 \rangle &= x_0^*(2) x_0(1) \left(\langle 0_2 | T | 0_1 \rangle \right. \\
&+ \sum_{i_2} \langle i_2 | T | 0_1 \rangle y_{i_2}^* + \sum_{i_1} \langle 0_2 | T | i_1 \rangle y_{i_1} \\
&\left. + \sum_{i_1, i_2} \langle i_2 | T | i_1 \rangle y_{i_2}^* y_{i_1} \right), \quad (19)
\end{aligned}$$

where the amplitudes x_0, y_i are obtained from (10) and (7) in the case of Rayleigh-Schroedinger expansion, or from (16) and (13) if we use the Brillouin-Wigner expansion.

The Bloch-Horowitz formalism³ is a generalization of the Brillouin-Wigner perturbation expansion, which is applied when there is a subset of states ($0, p, \dots$) which have to be simultaneously perturbed. Usually, these states are nearly degenerate. Eq. (12) is still valid, but now *both* (x_0) and (x_i) label the different components of the eigenvector corresponding to the unperturbed basic subset ($0, p, \dots$) and to the remaining unperturbed space (i, j, \dots), respectively. Previously this was the case only for (x_i).

Using (12), we again derive the amplitudes x_i as a function of the amplitudes of the basic subset x_0 , namely

$$x_i = \sum_0 y_{i0} x_0,$$

$$y_{i0} = - \sum_j \langle i | \frac{1}{H_0 + h' - E} | j \rangle h_{j0}. \quad (13')$$

We also obtain the Schroedinger equation in matrix form

$$\sum_p W_{0p}(E) x_p = E x_0,$$

$$W_{0p}(E) = \epsilon_0 \delta_{0p}$$

$$+ \sum_{n=1} \sum_{i,j,\dots,k}^{(n)} \frac{h_{0i} h_{ij} \dots h_{kp}}{(E - \epsilon_i)(E - \epsilon_j) \dots (E - \epsilon_k)}, \quad (20)$$

where the effective Hamiltonian $W(E)$ has only matrix elements within the basic subset. Equation (20) corresponds to a nonlinear eigenvalue problem

$$0 = |W_{0p}(E) - E \delta_{0p}|. \quad (14')$$

The eigenvectors are normalized in the whole space ($0, p, \dots, i, j, \dots$) (not in the basic subset). Using (13'), we obtain as in (15)

$$\begin{aligned}
1 &= \sum_{0,p} \left(\delta_{0p} + \sum_i y_{i0}^* y_{ip} \right) x_0^* x_p \\
&= \sum_{0,p} \left(\delta_{0p} - \frac{\partial}{\partial E} W_{0p}(E) \right) x_0^* x_p. \quad (15')
\end{aligned}$$

In this paper we have shown that there exist simple expressions for the square of the normalization coefficients, both in Rayleigh-Schroedinger and Brillouin-Wigner expansions, in terms of the derivative of the energy. The generalization to the Bloch-Horowitz formalism is made [Eq. (15')] in terms of the effective Hamiltonian.

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¹For instance, A. Messiah, *Mecanique Quantique* (Dunod, Paris, 1960), Vol. II, pp. 586.

²For instance, K. Kumar, *Perturbation Theory and the Nuclear Many-Body Problem* (North-Holland, Amsterdam, 1962), pp. 11.

³C. Bloch and J. Horowitz, *Nucl. Phys.* **8**, 91 (1958).