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Interpolation theory for quantum mechanics

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Abstract. We introduce methods for finding the energies and eigenstates of the Hamiltonian $H(\lambda) = (1 - \lambda)H_0 + \lambda H_1$ which smoothly interpolate between the limits $\lambda = 0, 1$.

1. Introduction

It is assumed the Hamiltonian

$$H(\lambda) = (1 - \lambda)H_0 + \lambda H_1 \quad (1)$$

succumbs to an exact treatment when $\lambda = 0$ or 1 . The problem is to devise general methods which interpolate between these special values where an exact analysis may no longer be possible.

We shall develop a perturbation expansion for the eigenstates and energy levels of $H(\lambda)$ in powers of $\lambda(1 - \lambda)$. This perturbation expansion is exact for $\lambda = 0$ or 1 and converges rapidly to the known result for a simple example we introduce to illustrate the theory.

It is important that H_0, H_1 have the same type of spectrum. Otherwise, we shall not be able to keep track of a particular energy level as λ varies. In this case, the interpolation will not be smooth.

The discussion centres on the ground state energy and assumes nondegeneracy. The necessary generalizations are straightforward.

2. Variational procedure for the ground state energy

The (normalized) eigenstates u_i, v_i and energies E_{0i}, E_{1i} of H_0, H_1 are known exactly. We shall write $E_{00} \equiv E_0, E_{10} \equiv E_1$.

Let $H(\lambda)$ have ground state $\psi(\lambda)$ with energy $E(\lambda)$. Then $\psi(0) = u_0, \psi(1) = v_0$.

Assume a normalized variational trial ground state of the form

$$\tilde{\psi}(\lambda) = f(\lambda)u_0 + g(\lambda)v_0. \quad (2)$$

We find that the numbers $f(\lambda), g(\lambda)$ which give the minimum expectation value of the energy satisfy the equation

$$(1 - \lambda)I g^2 + (1 - \lambda - \lambda M) f g - \lambda M I f^2 = 0 \quad (3)$$

where we have introduced

$$\begin{aligned}
 M_0 &= (v_0, H_0 v_0) - E_0 \\
 M_1 &= (u_0, H_1 u_0) - E_1 \\
 M &= M_1 / M_0 \\
 I &= (u_0, v_0) \neq 0.
 \end{aligned}
 \tag{4}$$

The normalization condition is

$$1 = f^2 + g^2 + 2gfI. \tag{5}$$

An estimate $\tilde{E}(\lambda)$ of the ground state energy is then

$$\tilde{E}(\lambda) = (1 - \lambda)(M_0 g^2 + E_0) + \lambda(M_1 f^2 + E_1). \tag{6}$$

To test the accuracy of the procedure we take

$$H_i = \frac{1}{2}(p^2 + a_i^2 q^2) \quad (i = 0, 1) \tag{7}$$

so that

$$H(\lambda) = \frac{1}{2}[p^2 + \{(1 - \lambda)a_0^2 + \lambda a_1^2\}q^2] \tag{8}$$

and compare the exact ground state energy

$$E(\lambda) = \frac{1}{2}\{(1 - \lambda)a_0^2 + \lambda a_1^2\}^{1/2} \tag{9}$$

with the estimate from the variational calculation.

It is a straightforward matter to write down the normalized ground state wavefunctions for the oscillators H_0 , H_1 and to evaluate M and I . Explicit expressions for f , g can now be found from (3) and (5) but these are somewhat messy. Instead, with $a_0 = 1$, $a_1 = 2$ to somehow represent the general case, the trial energy $\tilde{E}(\lambda)$ has been numerically calculated for $\lambda = 0(0.1)1$. Table 1 summarizes the computations and also includes estimates of the ground state energy to several orders of standard perturbation

Table 1. Summary of results of approximation schemes

λ	Exact energy	$\tilde{E}(\lambda)$	Interpolation expansion		Perturbation theory in powers of λ			
			$E_1(\lambda)$	$E_2(\lambda)$	$E^{(1)}(\lambda)$	$E^{(2)}(\lambda)$	$E^{(3)}(\lambda)$	$E^{(4)}(\lambda)$
0.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
0.1	0.5701	0.5706	0.5714	0.5700	0.5750	0.5794	0.5702	0.5701
0.2	0.6325	0.6338	0.6360	0.6318	0.6500	0.6275	0.6343	0.6317
0.3	0.6892	0.6910	0.6946	0.6879	0.7250	0.6744	0.6972	0.6843
0.4	0.7416	0.7435	0.7480	0.7399	0.8000	0.7100	0.7640	0.7235
0.5	0.7906	0.7922	0.7969	0.7888	0.8750	0.7344	0.8398	0.7410
0.6	0.8367	0.8379	0.8420	0.8352	0.9500	0.7475	0.9297	0.7247
0.7	0.8803	0.8811	0.8841	0.8795	1.0250	0.7494	1.0388	0.6589
0.8	0.9220	0.9223	0.9240	0.9216	1.1000	0.7400	1.1720	0.5240
0.9	0.9618	0.9619	0.9624	0.9617	1.1750	0.7194	1.3345	0.2965
1.0	1.0	1.0	1.0	1.0	1.2500	0.6875	1.5312	-0.0508

theory. Here $E^{(n)}(\lambda)$ is the n th order estimate of $E(\lambda)$ in a power series expansion about $\lambda = 0$.

We see that perturbation theory converges satisfactorily for $\lambda < 0.25$ but that convergence is slow beyond this value. Indeed, for $\lambda > \frac{2}{3}$ successive terms grow in size and the expansion is useless.

For $\lambda = \frac{1}{2}$, second order perturbation theory is about 7% out. Contrast this with the variational calculation which for less labour produces an estimate which differs 0.2% from the exact value.

3. Interpolation expansion of an arbitrary function

The variational calculation suffers because of the element of guesswork involved in setting up the trial ground state. There is, in fact, no reason why the exact state should look anything like (2) except near the values $\lambda = 0, 1$.

In the next section we derive a series expansion for $E(\lambda)$ (and $\psi(\lambda)$) in powers of $t = \lambda(1 - \lambda)$. Such an expansion exists for an arbitrary well behaved function.

We write

$$f(\lambda) = \tilde{f}_0 + t\tilde{f}_1 + t^2\tilde{f}_2 + \dots \tag{10}$$

where

$$\tilde{f}_i = (1 - \lambda)f_i + \lambda g_i \equiv [f_i, g_i]. \tag{11}$$

To determine the coefficients in the expansion, introduce the partial sum

$$f_n(\lambda) = \sum_{k=0}^n t^k \tilde{f}_k \tag{12}$$

and it follows that

$$f_{n+1} = \lim_{\lambda \rightarrow 0} \left(\frac{f(\lambda) - f_n(\lambda)}{\lambda^{n+1}(1 - \lambda)^{n+1}} \right) \quad g_{n+1} = \lim_{\lambda \rightarrow 1} \left(\frac{f(\lambda) - f_n(\lambda)}{\lambda^{n+1}(1 - \lambda)^{n+1}} \right). \tag{13}$$

An alternative procedure is to express $f(\lambda)$ as a power series in λ , and use

$$\begin{aligned} 1 &= [1, 1] \\ \lambda &= [0, 1] \\ \lambda^2 &= [0, 1] + t[-1, -1] \\ \lambda^3 &= [0, 1] + t[-1, -2] \\ \lambda^4 &= [0, 1] + t[-1, -3] + t^2[1, 1] \end{aligned}$$

to translate successive terms.

Finally, we note the multiplication formula

$$\begin{aligned} \tilde{f}_i \tilde{f}_j &= \{(1 - \lambda)f_i + \lambda g_i\} \{(1 - \lambda)f_j + \lambda g_j\} \\ &= (1 - \lambda)f_i g_j + \lambda f_j g_i - t(g_i - f_i)(g_j - f_j). \end{aligned} \tag{14}$$

4. Interpolation expansion for the ground state

Set

$$\begin{aligned}
 H(\lambda) &= \tilde{H} \\
 \psi(\lambda) &= \tilde{\psi}_0 + t\tilde{\psi}_1 + t^2\tilde{\psi}_2 + \dots \\
 E(\lambda) &= \tilde{E}_0 + t\tilde{E}_1 + t^2\tilde{E}_2 + \dots
 \end{aligned}
 \tag{15}$$

where

$$\tilde{E}_i = [A_i, B_i] \quad \tilde{\psi}_i = [\alpha_i, \beta_i]$$

may be assumed real.

To find the coefficients in these series we substitute into the Schrödinger equation $H(\lambda)\psi(\lambda) = E(\lambda)\psi(\lambda)$ and equate terms of the same power in t on both sides of the expansion.

Zeroth order contributions come from

$$\begin{aligned}
 \tilde{H}\tilde{\psi}_0 &= (1-\lambda)H_0\alpha_0 + \lambda H_1\beta_0 - t(H_1 - H_0)(\beta_0 - \alpha_0) \\
 \tilde{E}_0\tilde{\psi}_0 &= (1-\lambda)A_0\alpha_0 + \lambda A_1\beta_0 - t(B_0 - A_0)(\beta_0 - \alpha_0)
 \end{aligned}
 \tag{16}$$

and we find

$$(1-\lambda)H_0\alpha_0 + \lambda H_1\beta_0 = (1-\lambda)A_0\alpha_0 + \lambda A_1\beta_0.$$

This yields two eigenvalue equations

$$H_0\alpha_0 = A_0\alpha_0 \quad H_1\beta_0 = A_1\beta_0.
 \tag{17}$$

Since we are interested in the ground state we make the identification

$$\tilde{E}_0 = [E_0, E_1] \quad \tilde{\psi}_0 = [u_0, v_0].
 \tag{18}$$

First order contributions arise from $t\tilde{H}\tilde{\psi}_1$, $t\tilde{E}_1\tilde{\psi}_0$, $t\tilde{E}_0\tilde{\psi}_1$ and from (16). Using (14), neglecting second order terms in t gives

$$H_0\alpha_1 - (H_1 - H_0)(v_0 - u_0) = A_1u_0 + E_0\alpha_1 - (E_1 - E_0)(v_0 - u_0)
 \tag{19}$$

and

$$H_1\beta_1 - (H_1 - H_0)(v_0 - u_0) = B_1v_0 + E_1\beta_1 - (E_1 - E_0)(v_0 - u_0).
 \tag{20}$$

To determine A_1 and B_1 we take the innerproduct of (19), (20) with u_0, v_0 respectively, and find

$$A_1 = M_1 \quad B_1 = M_0.$$

Thus

$$E_1(\lambda) = (1-\lambda)(E_0 + tM_1) + \lambda(E_1 + tM_0)
 \tag{21}$$

correct to terms of first order in t .

Higher order corrections are determined in a similar manner using the orthogonality conditions $(u_i, u_j) = \delta_{ij} = (v_i, v_j)$. We find

$$\begin{aligned}
 E_2(\lambda) &= (1-\lambda) \left\{ E_0 + tM_1 + t^2 \left(2M_1 - M_0 - \sum_{j \neq 0} \frac{|(u_j, H_1 u_0)|^2}{E_{0j} - E_0} \right) \right\} \\
 &\quad + \lambda \left\{ E_1 + tM_0 + t^2 \left(2M_0 - M_1 - \sum_{j \neq 0} \frac{|(v_j, H_0 v_0)|^2}{E_{1j} - E_1} \right) \right\}.
 \end{aligned}
 \tag{22}$$

Also

$$\begin{aligned} \psi_1(\lambda) = (1-\lambda) & \left\{ u_0 + t \left(-v_0 + Iu_0 - \sum_{j \neq 0} \frac{u_j(u_j, H_1 u_0)}{E_{0j} - E_0} \right) \right\} \\ & + \lambda \left\{ v_0 + t \left(-u_0 + Iv_0 - \sum_{j \neq 0} \frac{v_j(v_j, H_0 v_0)}{E_{1j} - E_1} \right) \right\} \end{aligned} \quad (23)$$

provides an (un-normalized) first order estimate of the ground state $\psi(\lambda)$.

For $\lambda = \frac{1}{2}$, $E_1(\lambda)$, $E_2(\lambda)$ are approximately 0.8%, 0.2%, respectively, in error for the simple example of § 2. In this case, the results for the second order interpolation calculation are at least as good as the variational estimate.

5. Discussion

Methods have been presented which, under suitable conditions, give good estimates of the ground state energy for the interpolation problem. The basic assumptions fed into the theory such as the requirement that H_0 , H_1 have the same type of energy spectrum are no worse than standard perturbation theory.

Interpolation theory can be used to treat the general problem of two interacting systems. H_0 and H_1 represent the isolated systems. The approach is feasible when the two Hamiltonians have similar characteristics and it is unrealistic to regard one as a perturbation on the other.

Consider a binary alloy. A set $\{k\}$ of electrons interacts with species A, B of nuclei having charges Z_A , Z_B . The Hamiltonian for the combined system can be written

$$H = \sum_k \left(-\frac{1}{2} \nabla_k^2 - \sum_A \frac{Z_A}{r_{kA}} - \sum_B \frac{Z_B}{r_{kB}} \right) + V \quad (24)$$

where V is the electron-electron energy. Set

$$H_0 = \sum_k \left(-\frac{1}{2} \nabla_k^2 - \sum_A \frac{Z}{r_{kA}} \right) + V \quad (25)$$

$$H_1 = \sum_k \left(-\frac{1}{2} \nabla_k^2 - \sum_B \frac{Z}{r_{kB}} \right) + V$$

and note (1) with $\lambda = Z_B/Z$, $Z = Z_A + Z_B$. Interpolation theory gives an expansion in $\lambda(1-\lambda) = Z_A Z_B / Z^2$ about the single-species configurations.

For an application of the method to the diatom, see Byers-Brown and Power (1970).

Other developments in interpolation theory are envisaged in a Green function approach. We define

$$G(E, \lambda) = \frac{1}{E - H(\lambda)} \quad (26)$$

and expand in terms of $G_0(E) = 1/E - H_0$, $G_1(E) = 1/E - H_1$ and t . The result is

$$G(E, \lambda) = \{(1-\lambda)G_0 + \lambda G_1\} \left(\frac{1}{1 + t(H_1 - H_0)(G_1 - G_0)} \right) \quad (27)$$

and the well worn methods of perturbation theory can be employed to evaluate the second term to arbitrary order in t . But this is poaching material from a future paper.

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References

Byers-Brown W and Power J D 1970 *Proc. R. Soc. A* **317** 545–74