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Generalized Perturbation Theory: Quality of the First-Order Wave Function*

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A recently proposed version of generalized perturbation theory, in which the whole energy correction is taken care of in second order, is investigated with respect to the quality of its first-order wave function. It is demonstrated that the overlap of the wave function generated in this procedure with the exact solution is in most cases much closer to unity than those of the Rayleigh-Schroedinger or Brillouin-Wigner perturbation theories. Certain approximations, by means of which realistic systems become amenable to investigation within the presently discussed framework, are studied.

Key words: Generalized perturbation theory - First-order wave function

1. Introduction

The idea that a generalized perturbation theory can be formulated so as to include the Rayleigh-Schroedinger (RS) and Brillouin-Wigner (BW) theories as special cases, has been explicitly discussed by Young and March [1], Yaris [2] and Löwdin [3], and is implicit in the work of many others.

Although the formal aspects of this generalization have been studied in considerable detail, relatively little has been done towards applying it to actual computations. An interesting recent exception, in which some earlier references are discussed, is due to Cederbaum *et al.* [4–6], who have evaluated the extra parameters of their version of the generalized theory by means of a variational computation.

The presently reported investigation is concerned with the situation in which the energy is already known from some external theoretical or experimental source, but the wave function is not. This is a rather commonplace situation in atomic and molecular physics.

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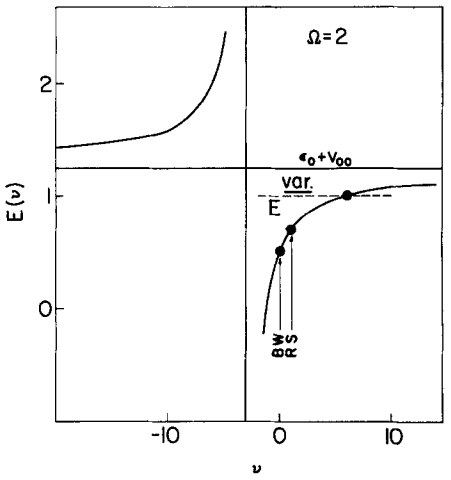

Fig. 1. Energy vs. ν for the ground state of the harmonic oscillator with a quadratic perturbation

Out of the general theory presented in Ref. [7] we shall only need the expression for the energy up to second order

$$E_\lambda^{(2)}(\nu) = \epsilon_0 + V_{00} - \sum_i{}' \frac{|V_{0i}|^2}{(\epsilon_i - E) - \nu(\epsilon_0 - E)} \tag{1}$$

and that for the wave function up to first order

$$\Psi_\lambda^{(1)}(\nu) = \psi^{(0)} - \sum_i{}' \frac{V_{0i}}{(\epsilon_i - E) - \nu(\epsilon_0 - E)} \psi_i. \tag{2}$$

Here λ is the strength parameter of the perturbation, $\{\epsilon_i, \psi_i\}$ are the eigenvalues and eigenfunctions of the unperturbed system, $E = E(\lambda)$ is the exact energy and ν is an additional parameter. BW corresponds to $\nu = 0$ and RS to $\nu = 1$.

Our program is as follows:
We shall solve the equation $E_\lambda^{(2)}(\nu_E) = E$ for $\nu_E = \nu_E(\lambda)$. The number of solutions of this equation is equal to the number of isolated singularities in $E_\lambda^{(2)}(\nu_E)$, i.e., the number of discrete states of the unperturbed Hamiltonian for which $V_{0i} \neq 0, i \neq 0$.

We shall investigate whether the quality of the wave function up to first order, which is obtained by using particular values of ν_E in Eq. (2) is actually superior to those corresponding to the standard (RS and BW) formulations. To this effect, the value of ν corresponding to the maximum of $|\langle \psi_\lambda^{(1)}(\nu)|\Psi_\lambda\rangle|^2$, to be denoted by ν_s, will be evaluated for several cases as a reference to the quality of the wave functions obtained with ν_E.

Furthermore, we shall consider certain approximations to ν_E, which may provide the possibility of studying realistic systems with a reasonable amount of effort, without knowledge of the exact energy.

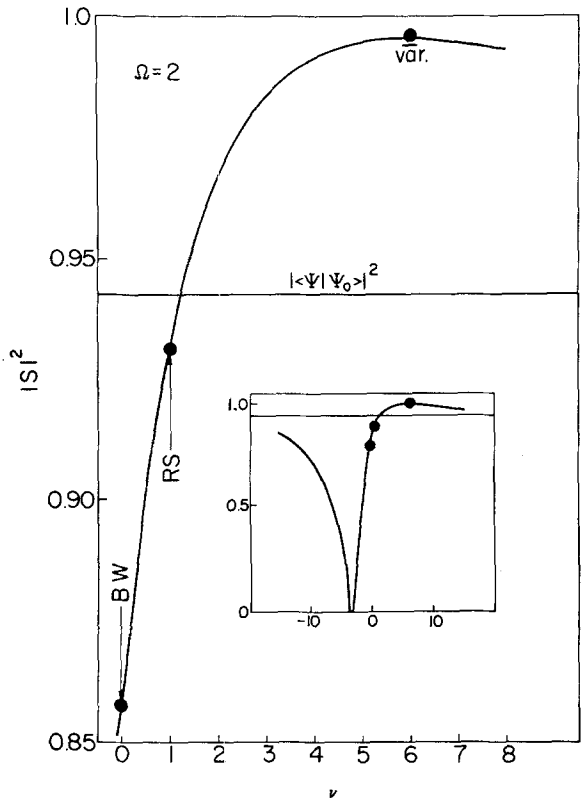

Fig. 2. Overlap vs. ν for the ground state of the harmonic oscillator with a quadratic perturbation

2. One Perturbing State

The simplest case consists of a state ψ_0 which has only one non-vanishing off-diagonal matrix element of the perturbation, with a state ψ_i. For this case one immediately obtains

$$\nu_E = \left[E - \epsilon_i - \frac{|V_{0i}|^2}{E - (\epsilon_0 + V_{00})}\right] \Big/ (E - \epsilon_0). \tag{3}$$

The overlap between the wave function up to first order and the exact wave function, considered as a function of ν, has two extrema, one of which, i.e.,

$$\nu_s = \left[E - \epsilon_i - V_{0i} \cdot \frac{\langle \Psi | \psi_0 \rangle}{\langle \Psi | \psi_i \rangle}\right] \Big/ (E - \epsilon_0) \tag{4}$$

corresponds to a maximum, whereas the second to a minimum. For this case the maximum overlap turns out to be equal to the best value achievable with the basis set employed, consisting of ψ_0 and ψ_i, according to Parseval's criterion. The minimum turns out to be zero.

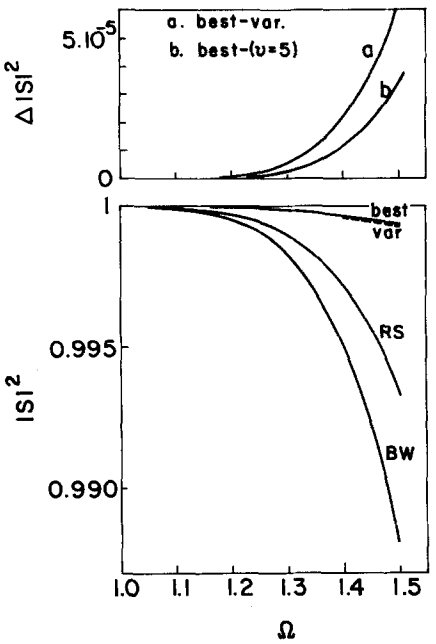

Fig. 3. Overlap in the various perturbation schemes for the harmonic oscillator with a quadratic perturbation

2.1. Examples

2.1.1. Ground State of the Harmonic Oscillator with a Linear Perturbation

Here

$$H_0 = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\omega^2}{2}x^2 \qquad \text{and} \qquad V = \lambda x,$$

furthermore,

$$V_{0i} = \delta_{1,i} \cdot \lambda\sqrt{2\omega}, \qquad E = \frac{\omega}{2} - \frac{\lambda^2}{2\omega^2} \qquad \text{and} \qquad \frac{\langle\Psi \mid \psi_0\rangle}{\langle\Psi \mid \psi_1\rangle} = -\sqrt{2/\omega}/\mu$$

where $\mu = \lambda/\omega^2$. Hence, $\nu_E = \nu_S = 1$, i.e., RS is the best scheme.

2.1.2. Ground and First Excited State of the Harmonic Oscillator with a Quadratic Perturbation

The unperturbed Hamiltonian is as above but $V = (\lambda/2)x^2$. For the ground state one has

$$E = \frac{\Omega}{2}, \qquad V_{0i} = \frac{\lambda}{4\omega} \cdot (\delta_{i0} + \sqrt{2} \cdot \delta_{i,2}) \qquad \text{and} \qquad \frac{\langle\Psi \mid \psi_0\rangle}{\langle\Psi \mid \psi_2\rangle} = (\Omega + \omega)\sqrt{2}/(\omega - \Omega)$$

where $\Omega^2 = \omega^2 + \lambda$, i.e., Ω is the frequency of the perturbed oscillator.

Hence, $\nu_E = \nu_S = 5 + (\Omega - \omega)/\omega$. In this case ν turns out to be far away from the $(0, 1)$ range corresponding to the two classical schemes.

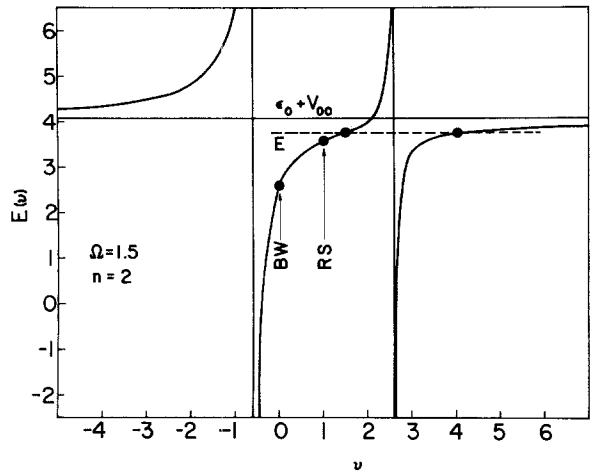

Fig. 4. Energy vs. ν for the second excited state of the harmonic oscillator with a quadratic perturbation

The dependence of the energy up to second order, and of the overlap of the exact wave function with that up to first order, on ν, is shown in Figs. 1 and 2, respectively, for a perturbation of a fixed strength. The dependence of the best overlap on the strength of the perturbation is shown in Fig. 3.

Figs. 2 and 3 indicate that the wave function generated with ν_E $(= \nu_s)$ has a fairly high overlap with the exact wave function even for large perturbations, for which RS and BW perform quite poorly. A variational computation was carried out using the unperturbed wave functions ψ_0 and ψ_2 as a basis. For the case presently discussed this kind of variational computation coincides with the method of Cederbaum *et al.* [4-6]. The variational energy and the overlap of the corresponding wave function with the exact one are indicated in Figs. 1 and 3. The variational wave function has a (slightly) smaller overlap than $\psi(\nu_E)$.

For the first excited state one similarly obtains

$$\nu_E = \nu_s = \tfrac{7}{3} + \frac{\Omega - \omega}{3\omega}.$$

The equality of ν_E and ν_s in all the three examples discussed is of no general validity, as further examples will indicate.

3. Two Perturbing States

The explicit expressions for ν_E and ν_s are already too cumbersome in this case to be worth presenting in their general forms. The main new aspect of the situation presently discussed is the fact that there are two solutions to the equation for ν_E, for any value of λ. It is very plausible that one of these solutions is superior from the point of view of criteria such as the overlap with the exact wave function, the corresponding variational energy or the width of the Hamiltonian. It will be very important from a practical point of view to have an *a priori* clue to the identification of this solution.

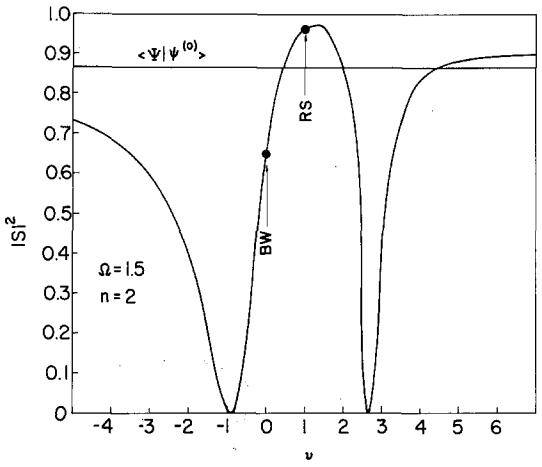

Fig. 5. Overlap vs. ν for the second excited state of the harmonic oscillator with a quadratic perturbation

3.1. Examples

3.1.1. Excited States of the Harmonic Oscillator with a Quadratic perturbation

The Hamiltonian is the same as that in Sect. 2.1.2 but now we are interested in the excited states with at least two quanta. The nth state ($n > 2$) is connected in first order with the states $n + 2$ and $n - 2$ as follows:

$$V_{n,n+2} = \lambda \cdot \sqrt{(n+1)(n+2)}/(4\omega); \qquad V_{n,n-2} = \lambda \cdot \sqrt{(n-1)n}/(4\omega).$$

The dependence of the energy and of the overlap on ν is shown in Figs. 4 and 5, respectively. Out of the two values of ν_E shown in Fig. 4 the one on the "canonical branch" (containing RS on it) is closer to the value ν_s corresponding to the maximum overlap.

3.1.2. Ground State of the Harmonic Oscillator with a Quartic Perturbation

The unperturbed Hamiltonian is as in the previous section, but the perturbation is $V = \lambda x^4$. This is our first non-trivial example, at least in the sense that the exact solution is not analytically available.

In order to compute the exact energy and the overlap between the first order and the exact wave function, we solve the problem variationally, using the set of eigenstates of the unperturbed harmonic oscillator. Increasing the size of the basis set we reach convergence to at least 7 decimal places in the energy and 4 decimal places in the normalized coefficients of ψ_0, ψ_2 and ψ_4, which are the only coefficients needed to compute the overlap with the first-order wave function. These accuracies are obtained with basis sizes of about 10 harmonic functions.

The matrix elements of the perturbation are given by Biswas *et al.* [8]. As in the previous case, the value of ν_E belonging to the canonical branch corresponds to a higher overlap wave function than the other solution. The overlap of $\psi(\nu_E)$ with the exact wave function is almost as good as the best overlap and much closer to unity than that of RS and BW (Fig. 6). The energy error in the various perturbation schemes ($\Delta E = E(\nu) - E_{\text{exact}}$) is shown in Fig. 7.

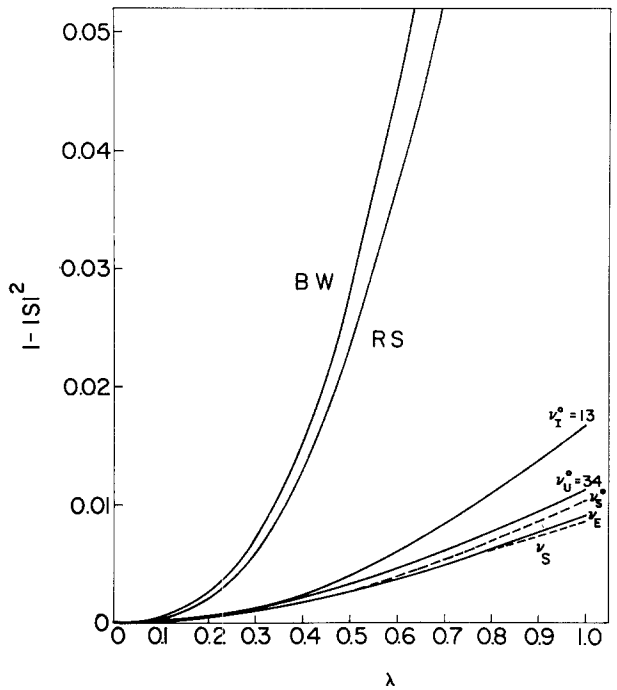

Fig. 6. Overlap in the various perturbation schemes for the harmonic oscillator with a quartic perturbation

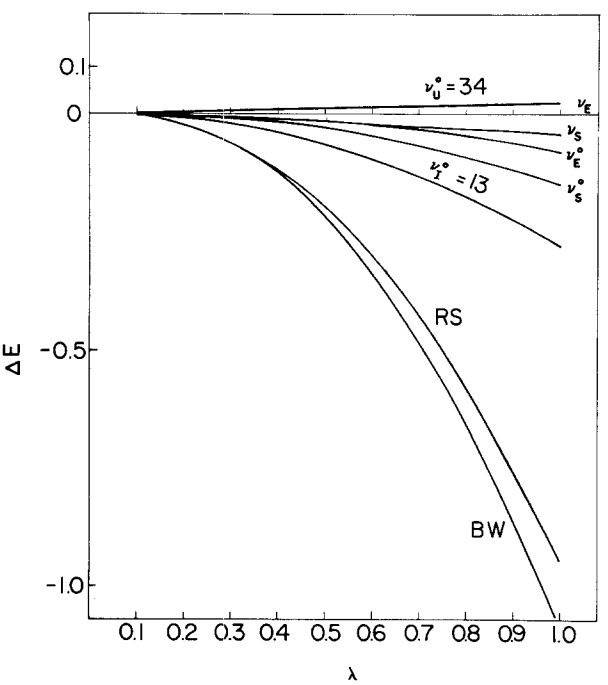

Fig. 7. Energy error in the various perturbation schemes for the harmonic oscillator with a quartic perturbation

4. More General Systems: The Two-Centre δ-Function Hamiltonian

The one-dimensional δ-function Hamiltonian [9]

$$H_0 = -\frac{d^2}{dx^2} - 2 \cdot \delta(x - a)$$

has a spectrum consisting of one bound state

$$\phi_0 = \exp(-|x - a|); \qquad \epsilon_0 = -1$$

and a continuum whose Green's function is

$$\Gamma(x, y) \equiv \sum_n{}' \frac{|\phi_n\rangle\langle\phi_n|}{-\beta^2 - \epsilon_n} = \exp[-(|x - a| + |y - a|)]/(\beta^2 - 1)$$
$$- \exp[-\beta(|x - a| + |y - a|)]/[2\beta(\beta - 1)] - \exp(-\beta|x - y|)/(2\beta). \tag{5}$$

Introducing $V = -2\lambda \cdot \delta(x + a)$ as the perturbation, we get the two-centre δ-function Hamiltonian whose ground state energy and eigenfunction are given by $E = -\gamma^2$ where $(\gamma - 1) \cdot (\gamma - \lambda) = \lambda \exp(-4\gamma a)$ and $\psi = A \cdot \exp(-\gamma|x - a|) + \exp(-\gamma|x + a|)$

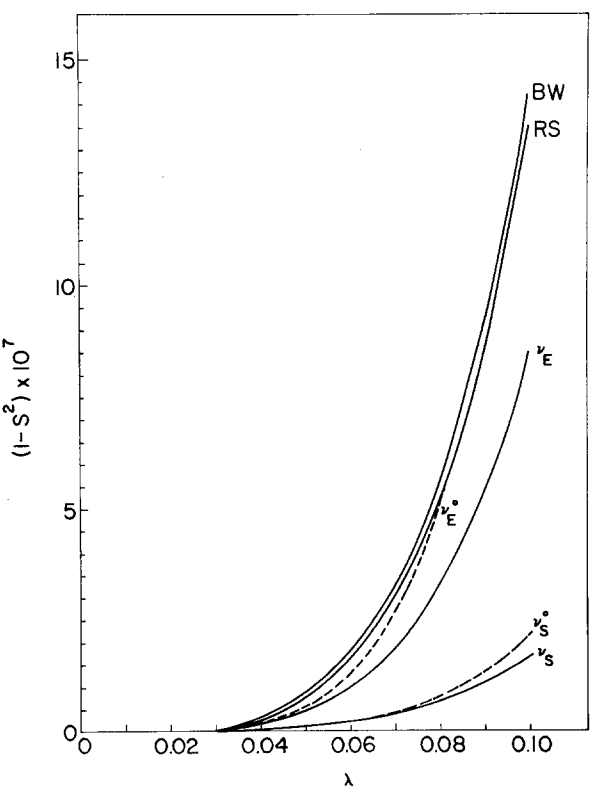

Fig. 8. Overlap for the two-centre δ-function

where $A = \exp(-2\gamma a)/(\gamma - 1)$. The perturbation theory corrections are

$$\epsilon^{(1)} = -2\lambda \cdot \exp(-4a)$$

$$\epsilon^{(2)}(\nu) = -4\lambda^2 \cdot \exp(-4a) \cdot \{1/(2\beta) + [\exp(-4\beta a)(2\beta) - \exp(-4a)/(\beta + 1)]/(\beta - 1)\}$$

and

$$\psi^{(0)} + \psi^{(1)} = A_p \cdot \exp(-|x - a|) + B_p \cdot \exp(-\beta|x - a|) + C_p \cdot \exp(-\beta|x + a|)$$

where

$$A_p = (\beta - 1) - 2\lambda \cdot \exp(-4a)/(\beta + 1)$$

$$B_p = \lambda \cdot \exp[-2a \cdot (1 + \beta)]/\beta$$

$$C_p = \lambda(\beta - 1) \cdot \exp(-2a)/\beta$$

$$-\beta^2 = E + \nu(\epsilon_0 - E).$$

Using these results and overlap integrals of the form

$$\int_{-\infty}^{\infty} \exp[-\alpha|x - a| - \beta|x + a|]\, dx = \begin{cases} 2[\alpha \cdot \exp(-2\beta a) - \beta \cdot \exp(-2\alpha a)]/(\alpha^2 - \beta^2) & \text{for } \alpha \neq \beta \\ (1 + 2\alpha a)\exp(-2\alpha a)/\alpha & \text{for } \alpha = \beta \end{cases}$$

the results presented in Fig. 8 were evaluated, for $a = 1$. The main result to be pointed out is that for a sufficiently large perturbation $\psi(\nu_E)$ ceases to be a better approximation to the exact wave function than RS and BW.

5. Asymptotic Values of ν_E and ν_s for Small Perturbations

As a first attempt to formulate a starting point for the generalized perturbation theory, which does not depend on complete knowledge of the perturbed energy, we shall now study the behaviour of ν_E and ν_s for small perturbations. This will enable us to derive some approximate but simple expressions for them. Let $\nu_E^0 = \lim_{\lambda \to 0} \nu_E$ and $\nu_s^0 = \lim_{\lambda \to 0} \nu_s$.

It is shown in the Appendix that

$$\nu_E^0 = \sum_{j,k}{}' \frac{V_{0j}V_{jk}V_{k0}}{(\epsilon_0 - \epsilon_j)(\epsilon_0 - \epsilon_k)} \Bigg/ \left[V_{00} \cdot \sum_i{}' \frac{|V_{0i}|^2}{(\epsilon_0 - \epsilon_i)^2}\right] \tag{6}$$

and

$$\nu_s^0 = \sum_{j,k}{}' \frac{V_{0j}V_{jk}V_{k0}}{(\epsilon_0 - \epsilon_j)^3(\epsilon_0 - \epsilon_k)} \Bigg/ \left[V_{00} \cdot \sum_i{}' \frac{|V_{0i}|^2}{(\epsilon_0 - \epsilon_i)^4}\right]. \tag{7}$$

Introducing the modified Green's function

$$\Gamma = \sum_i{}' \frac{|i\rangle\langle i|}{\mu - \epsilon_i}$$

we get

$$\Gamma^{(n)} \equiv \frac{\partial^n \Gamma}{\partial \mu^n}\bigg|_{\epsilon_0} = (-1)^n \cdot n! \cdot \sum_i{}' \frac{|i\rangle\langle i|}{(\epsilon_0 - \epsilon_i)^{n+1}}$$

with these derivatives of the Green's function we can write

$$\nu_E^0 = -\langle 0|V\Gamma^{(0)}V\Gamma^{(0)}V|0\rangle/(V_{00}\cdot\langle 0|V\Gamma^{(1)}V|0\rangle \tag{8}$$

and

$$\nu_S^0 = -3\langle 0|\Gamma^{(2)}V\Gamma^{(0)}V|0\rangle/(V_{00}\cdot\langle 0|V\Gamma^{(3)}V|0\rangle)\cdot \tag{9}$$

5.1. Approximations to the Asymptotic Expressions

The approximations introduced in the present section are hoped to provide some starting point for the application of the generalized perturbation theory to realistic systems.

5.1.1. Unsöld Type Approximation

The expressions for ν_E^0 and ν_S^0 contain energy denominators in a manner which makes an Unsöld type approximation particularly attractive. This is so because the constant energy difference taken outside of the summations prior to application of the closure relations appears, raised to the same power, in both the numerator and the denominator.

The result for both the energy and the overlap is

$$\nu_U^0 = \frac{1}{V_{00}} \cdot \frac{(V^3)_{00} - 2V_{00}\cdot(V^2)_{00} + (V_{00})^3}{(V^2)_{00} - (V_{00})^2}. \tag{10}$$

In this approximation the reduced weights of the higher energy terms are neglected as a consequence of replacing all energy differences by a constant. This is probably more severe for the overlap than for the energy, the energy denominators being of forth power in the former compared to second power in the latter. It therefore seems likely that ν_E^0 is better approximated by ν_U^0 than ν_S^0.

5.1.2. Single Term Approximation

As Unsöld's approximation neglects the differences in weights of the different terms, due to the energy denominators, it may be instructive to compare it with the other extreme approximation, in which we assume that only one state, most likely the one nearest the state we are interested in, contributes to the sums over states in ν_E^0 and ν_S^0. In this approximation $\nu_I^0 = V_{ii}/V_{00}$, where i is the only contributing state. In view of the discussion following the introduction of the Unsöld approximation it seems likely to expect the present approximation to be closer to ν_S^0 than to ν_E^0. This conjecture and the corresponding one for the Unsöld approximation are studied through the following examples.

5.2. Examples of the Asymptotic Expressions and Their Approximations

5.2.1. One Perturbing State

Denoting the state of interest by ψ_0 and the perturbing state by ψ_1 one obtains from the general expression

$$\nu^0 \equiv \nu_E^0 = \nu_S^0 = \nu_I^0 = \nu_U^0 = \frac{V_{11}}{V_{00}} .$$

For the ground state of the harmonic oscillator with a harmonic perturbation $\nu^0 = 5$ and for the first excited state $\nu^0 = 7/3$, in agreement with the results in Sect. 2.1.2. The upper part of Fig. 3 indicates that for the ground state of the harmonic oscillator with a quadratic perturbation the overlap of $\psi(\nu^0)$ with the exact wave function is better than that of the variational wave function, and practically identical with the best overlap as far as the comparison with RS and BW is concerned.

5.2.2. Two Perturbing States

If the two perturbing states ψ_i and ψ_j are situated with respect to the state of interest, ψ_0, so that $\epsilon_0 - \epsilon_i = \epsilon_j - \epsilon_0$ then

$$\nu^0 \equiv \nu_E^0 = \nu_S^0 = \frac{V_{0i}^2 \cdot V_{ii} + V_{0j}^2 \cdot V_{jj} - 2V_{0i} \cdot V_{ij} \cdot V_{j0}}{V_{00} \cdot (V_{0i}^2 + V_{0j}^2)} .$$

For the excited states of the harmonic oscillator with a harmonic perturbation one obtains $\nu^0 = 1 + 4/(n^2 + n + 1)$, which for $n > 2$ is already close enough to $\nu = 1$ to indicate that the improvement over the RS scheme cannot be expected to be substantial.

For the ground state of the harmonic oscillator with a quartic perturbation one obtains $\nu_E^0 = 23\frac{10}{13}$, $\nu_S^0 = 19\frac{2}{7}$, $\nu_I^0 = 13$ and $\nu_U^0 = 34$. The ordering $\nu_I^0 < \nu_S^0 < \nu_E^0 < \nu_U^0$ is in rough agreement with the comments made in the general discussion following the introduction of the Unsöld and single term approximations. Figs. 6 and 7 show that using ν_E^0, ν_S^0 or even the approximations to them (ν_U^0 and ν_I^0) one obtains considerably improved results, in comparison with the conventional RS and BW schemes.

5.2.3. The Two-Centre δ-Function Hamiltonian

Using the modified Green's function, Eq. (5), and the expressions for ν_E^0 and ν_S^0, Eqs. (8)-(9), one gets $\nu_E^0 = 60.0$ and $\nu_S^0 = 37.6$, in agreement with the extrapolation to $\lambda = 0$ of the values evaluated numerically. Overlaps are presented in Fig. 8.

6. Discussion

The main conclusion emerging out of the results presented is that using ν_E, and even ν_E^0 or one of the approximations to it (ν_U^0 or ν_I^0) in order to modify the first-order wave function is a useful procedure generating an improved wave function without really investing a significant amount of extra effort in comparison with the standard formulations of perturbation theory.

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Appendix: Derivation of the Asymptotic Expressions ν_E^0 and ν_s^0

We shall write the second-order energy in the form

$$E^{(2)} = -\sum_i{}' \frac{|V_{0i}|^2}{\epsilon_i - E} \cdot \frac{1}{1 - \nu \cdot \xi_i}$$

where $\xi_i = (\epsilon_0 - E)/(\epsilon_i - E)$. Clearly, as $\lambda \to 0$, $\xi_i \to 0$, so that provided that ν_E^0 is finite one can write

$$E^{(2)} \simeq E_{\mathrm{BW}}^{(2)} + \nu_E^0 \cdot V_{00} \cdot \sum_i{}' \frac{|V_{0i}|^2}{(\epsilon_i - \epsilon_0)^2} \cdot$$

Equating the second term to the third-order BW term one obtains Eq. (6). Denoting by S the overlap between the exact and the normalized first-order wave function we get

$$|S|^2 = |S_0|^2 \cdot \frac{\left[1 + \sum_i{}' \sigma_i \cdot \frac{V_{0i}}{E - \epsilon_i} \cdot \frac{1}{1 - \nu\xi_i}\right]^2}{1 + \sum_i{}' \left(\frac{V_{0i}}{\epsilon_i - E}\right)^2 \cdot \frac{1}{(1 - \nu\xi_i)^2}}, \qquad \text{where } S_0 = \langle \Psi \mid \psi_0 \rangle$$

and $\sigma_i = \langle \Psi \mid \psi_i \rangle / S_0$.

For small perturbations one can approximate this through the following steps

$$|S|^2 \simeq |S_0|^2 \cdot \left[1 + 2 \sum_i{}' \sigma_i \frac{V_{0i}}{E - \epsilon_i} \cdot \frac{1}{1 - \nu\xi}\right] \cdot \left[1 - \sum_i{}' \left(\frac{V_{0i}}{E - \epsilon_i}\right)^2 \cdot \frac{1}{(1 - \nu\xi_i)^2}\right]$$

$$\simeq |S_0|^2 \cdot \left\{1 + \sum_i{}' \frac{V_{0i}}{E - \epsilon_i} \cdot \left[\frac{2\sigma_i}{1 - \nu\xi_i} - \frac{V_{0i}}{E - \epsilon_i} \cdot \frac{1}{(1 - \nu\xi_i)^2}\right]\right\}$$

$$\simeq |S_0|^2 \cdot (1 + A + B \cdot \nu + C \cdot \nu^2)$$

where

$$A = \sum_i{}' \frac{V_{0i}}{\epsilon_0 - \epsilon_i} \cdot \left(2\sigma_i - \frac{V_{0i}}{E - \epsilon_i}\right)$$

$$B = \sum_i{}' \frac{V_{0i}}{(\epsilon_0 - \epsilon_i)^2} \cdot 2\left(\sigma_i - \frac{V_{0i}}{E - \epsilon_i}\right) \cdot V_{00}$$

$$C = \sum_i{}' \frac{V_{0i}}{(\epsilon - \epsilon_i)^3} \cdot \left(2\sigma_i - 3\frac{V_{0i}}{E - \epsilon_i}\right) \cdot V_{00}^2 \cdot$$

The maximum overlap is obtained for $\nu_s = -B/2C$. In order to obtain σ_i we write the exact wave function in terms of its RS expansion up to second order, i.e.,

$$\Psi = \psi_0 + \sum_j{}' \frac{V_{0j}}{\epsilon_0 - \epsilon_j}\psi_j + \sum_{j,k}{}' \frac{V_{kj}V_{j0}}{(\epsilon_0 - \epsilon_j)(\epsilon_0 - \epsilon_k)}\psi_k - V_{00}\cdot\sum_j{}' \frac{V_{j0}}{(\epsilon_0 - \epsilon_j)^2}\psi_j - \tfrac{1}{2}\psi_0 \cdot \sum_j{}' \frac{|V_{0i}|^2}{(\epsilon_0 - \epsilon_j)^2}\cdot$$

Using this representation of the exact wave function we get

$$\sigma_i \simeq \frac{\dfrac{1}{\epsilon_0 - \epsilon_i}\cdot\left[V_{0i}\cdot\left(1 - \dfrac{V_{00}}{\epsilon_0 - \epsilon_i}\right) + \sum_j{}' \dfrac{V_{ij}V_{j0}}{\epsilon_0 - \epsilon_j}\right]}{1 - \tfrac{1}{2}\sum_j{}' \dfrac{|V_{0j}|^2}{(\epsilon - \epsilon_j)^2}}$$

$$\simeq \left[V_{0i}\left(1 - \frac{V_{00}}{\epsilon_0 - \epsilon_i}\right) + \sum_j{}' \frac{V_{ij}V_{i0}}{\epsilon_0 - \epsilon_j}\right] \Big/ (\epsilon_0 - \epsilon_i).$$

We also need

$$\frac{V_{0i}}{E - \epsilon_i} \simeq \frac{V_{0i}}{\epsilon_0 - \epsilon_i}\left(1 - \frac{V_{00}}{\epsilon_0 - \epsilon_i}\right)$$

to obtain Eq. (7).

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