Excited bound state logarithmic perturbation theory without nodes

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Abstract. The logarithmic perturbation theory is modified slightly in order to deal with excited states. Instead of considering a real wavefunction describing the physical stationary state, we consider a complex wavefunction at the same energy, by mixing in the ghost state. For excited bound states, the former has nodes, while the latter is guaranteed not to have any nodes, and can be represented simply as $\exp(-G)$, to which the logarithmic perturbation method can be applied in a straightforward manner. The physical entities (the energy corrections) are independent of the amount of mixing of the ghost state. The connection to the Green function method is also shown. The freedom to mix in the ghost state allows us to justify an *ad hoc* approach whereby the simple version of the logarithmic perturbation theory is applied to excited bound states. The formalism is illustrated with simple examples.

1. Introduction

Bound state perturbation theory has played an important role in the study of a wide range of problems since the introduction of quantum mechanics. By considering the logarithm of the wavefunction instead of the wavefunction itself, the non-relativistic Schrödinger equation for bound states is transformed to the nonlinear Ricatti form [1-5]. Upon a perturbation expansion, the differential equations that determine the perturbative corrections become linear again, order by order [4]. These linear differential equations are first order. For general three-dimensional problems, these linear differential equations involve the divergence of a vector, that in turn is the gradient of a scalar field [5]. Thus effectively, one still deals with a second-order differential equation, though no longer an eigenvalue problem. However, for one-dimensional problems, this transformation, via the logarithm of the wavefunction and its derivative, provides a very convenient way to transform the second-order differential equation into two uncoupled first order differential equations, enabling the perturbative solutions to be obtained by quadratures, order by order [4]. We refer to this as the fundamental logarithmic perturbation method.

For excited bound states in one dimension, the wavefunction has zeros and its logarithm is singular, so that the simple version of logarithmic perturbation theory breaks down. A way to bypass this difficulty has been suggested earlier [4]. In this procedure (the node factorization method) the nodes are first factorized and then the logarithm of the remaining non-zero envelope is taken. The perturbative shifts in the

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nodal positions, the energies, and the logarithm of the wavefunction envelope are then obtainable in quadratures. But this method requires exact knowledge of the positions of the nodes in the unperturbed wavefunction and that their perturbative shifts be accounted for order by order. Except for the low-lying excited states, this knowledge is generally hard to obtain, even though the exact analytic form of the unperturbed wavefunction is available. For example, the zeros of a high-order polynomial (Hermite, Laguerre, etc) are not easy to find. Thus, even though a valid prescription to deal with excited bound state perturbations in one dimension is available, it is difficult to carry out in practice. The purpose of the present paper is to introduce an alternative method to bypass the nodal difficulty. Instead of considering a real wavefunction (which contains zeros) describing the stationary state, we consider a complex function at the same energy, carrying a non-zero probability flux. The real part of this complex wavefunction is the physical state, while the imaginary part is given by σ times the ghost state (the second solution, usually not normalizable). This complex wavefunction is guaranteed not to have any zeros and thus has a regular logarithm. The logarithmic perturbation method can then be applied in a straightforward manner. We shall show that the perturbative corrections to the energy (the physical entity) is independent of σ, the amount of mixing of the ghost state wavefunction, and we shall demonstrate explicitly the equivalence to the Green function method, up to the third order. We also justify an *ad hoc* approach whereby the usual logarithmic perturbation theory can be applied to excited states without modification.

Wentzel [1] seems to be the first to use the logarithmic transformation to Ricatti form in the study of the perturbative Stark shifts in hydrogen in parabolic coordinates. Since then, the technique of logarithmic perturbation expansion has been rediscovered and improved upon over and over again [2-15]. The logarithmic perturbation method is not the only one that bypasses the use of the Green function or the sum over intermediate states. Other direct attempts to obtain the perturbative corrections to the wavefunction as the solution of inhomogeneous multidimensional differential equations were also made by Schrödinger [16], Podolsky [17] and Sternheimer [18]. An elegant method of calculating sum rules was also introduced by Dalgarno and Lewis [19]. A perturbation method to calculate the energy corrections without calculation of the perturbed wavefunctions by use of the hypervirial relations was introduced by Swenson and Danforth [20] for the anharmonic oscillator and applied to the hydrogen atom by Killingbeck [21] and by Grant and Lai [22].

The complexity of the application of logarithmic perturbation expansion obviously increases with the dimensionality of the system. As pointed out earlier, the perturbative corrections are no longer obtainable in quadrature form when the perturbation is non-trivial as the differential equations involve the divergence of a vector, that is in turn the gradient of a scalar field [5]. Nevertheless, in certain situations, suitable separation of variables can be used to obtain the perturbative corrections as solutions to these differential equations [23]. An example is found in the calculation of hydrogenic dipole sum rule [24]. Recently, we have succeeded in extending this calculation of hydrogenic multipole sum rules to arbitrary multipolarity and arbitrary dimensions [25].

In section 2, we shall develop our formalism of using complex wavefunction in excited bound state logarithmic perturbation theory. In section 3, we shall obtain explicit formulae for the energy corrections. We shall show that the physical entities are independent of the amount of mixing of the ghost state and establish the equivalence of the present method with the Green function method, up to and including the third order. In section 4, we illustrate our formalism with the quartic anharmonic oscillator.

We show that the ghost state mixing method gives an unambiguous answer (in section 4.2). The straightforward application of logarithmic perturbation theory (i.e. without first factoring out the zeros of the unperturbed wavefunction) is clearly invalid for excited states, leading to formally divergent expressions whose values are ambiguous. This will be seen explicitly in section 4.1. Yet it has been found [20] that by implicitly adopting an *ad hoc* prescription for dealing with such ambiguous expression, the straightforward perturbation method miraculously gives the correct energy correction, at least to second order. This prescription is spelled out precisely in section 4.1 and proved to be correct in section 5. The proof shows that a small but non-zero admixture of the ghost state has the simple effect of pushing the nodal singularities slightly off the real axis, thus regulating the ambiguous expressions. Some concluding remarks are given in section 6. An explicit example is given in the appendix to demonstrate the independence of the energy shifts on the amount of ghost state mixing for a stretched square well.

2. Formalism

2.1. Defining functions

Consider a one-dimensional system defined by the Hamiltonian

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) + \lambda U(x) = H_0 + \lambda U(x) \tag{2.1}$$

where λU is the perturbing potential and λ is a formal small parameter. In order to mimic a radial problem, we shall assume that the particle is restricted to the positive halfline by an infinite potential $V(x) + \lambda U(x) = \infty$ for $x < 0$. Generalization to a full line problem is straightforward. The wavefunction satisfies

$$H\Phi = E\Phi \tag{2.2}$$

where the physical solution and the value of the energy E are selected by the boundary condition

$$\Phi(0) = 0 \tag{2.3a}$$

$$\Phi(\infty) = 0. \tag{2.3b}$$

The eigenvalue equation (2.2) admits a second solution, the ghost state $\chi(x)$, related to $\Phi(x)$ via [26]

$$\chi(x) = -\Phi(x) \int^x \frac{\mathrm{d}y}{\Phi(y)^2} \tag{2.4}$$

where the normalization has been chosen so that the Wronskian satisfies

$$W \equiv \Phi'(x)\chi(x) - \Phi(x)\chi'(x) = 1 \tag{2.5}$$

and where $' = \mathrm{d}/\mathrm{d}x$. Note that the lower limit in (2.4) is not specified. This means that one can mix any amount of Φ in χ without upsetting the Wronskian property. In the example of the anharmonic oscillator to be considered in section 4 below, it seems natural to choose χ and Φ to have opposite parities. Instead of dealing with the physical state Φ or the ghost state χ, we shall choose to consider the auxiliary function ψ

$$\psi \equiv \Phi + \mathrm{i}\sigma\chi \tag{2.6}$$

where σ is an arbitrary real and non-zero constant. It is obvious that ψ does not have any zero, because for ψ to vanish, it is necessary for both Φ and χ to vanish, which violates (2.5). Hence, a logarithmic perturbation expansion on ψ can be developed, in analogy with the ground state case discussed by Aharonov and Au [4]. Specifically we have

$$\psi \equiv \exp(-G) \qquad g \equiv G' \qquad\qquad (2.7)$$

and we expand G, E and g in power series in λ:

$$G = \sum_i \lambda^i G_i \qquad E = \sum_i \lambda^i E_i \qquad g = \sum_i \lambda^i g_i. \qquad (2.8)$$

Since ψ is the solution to a second-order differential equation, we can fix

$$\psi(0) = \psi_0(0) \qquad \psi'(0) = \psi_0'(0) \qquad\qquad (2.9a)$$

where the subscript zero indicates the unperturbed state. For such a choice of boundary conditions, we have

$$G_i(0) = 0 = g_i(0) \qquad \text{for all } i \neq 0. \qquad\qquad (2.9b)$$

Then proceeding as in [4], we get

$$g_n(x) = h_n(x)/\rho(x) \qquad\qquad (2.10a)$$

$$h_n(x) \equiv 2 \int_0^x F_n(y)\rho(y) \, dy \qquad\qquad (2.10b)$$

$$F_n(y) \equiv E_n - \tilde{U}_n(y) \qquad\qquad (2.10c)$$

where

$$\rho(x) = \psi_0(x)^2 \qquad\qquad (2.11)$$

$$\tilde{U}_1(x) = U(x) \qquad\qquad (2.12a)$$

$$\tilde{U}_n(x) = -\frac{1}{2} \sum_{i=1}^{n-1} g_i(x)g_{n-i}(x) \qquad n > 1 \qquad\qquad (2.12b)$$

$$= -\frac{1}{2\rho^2(x)} \sum_{i=1}^{n-1} h_i(x)h_{n-i}(x) \qquad n > 1. \qquad\qquad (2.12c)$$

For $n > 1$, $\tilde{U}_n$ depends only on lower-order quantities. There are only two differences from the treatment in [4]: the lower limit in (2.10b) is $x = 0$, where the boundary condition is imposed, rather than $x = -\infty$; also $\tilde{U}_n$ may now be complex for $n > 1$.

2.2. Quantization

Equation (2.10) allows us to find $g_n(x)$ once E_n is given, but E_n is not yet known. This is no surprise since we have not yet imposed the condition that the state in question is a bound state. Let the unperturbed wavefunction have the asymptotic behaviour

$$\psi_0 \sim -i\alpha \, e^{W(x)} \qquad x \to \infty \qquad\qquad (2.13)$$

where the reason for inserting $-i$ will become apparent, and

$$W(x) = \int^x dy\{2[V(y) - E_0]\}^{1/2} > 0 \qquad\qquad (2.14)$$

is the WKB exponent. Of course there is also a sub-asymptotic term going like e^{-W}. The unperturbed physical solution then behaves as

$$\Phi_0 = \operatorname{Re} \psi_0 \sim (\operatorname{Im} \alpha) \, e^{W(x)} \qquad x \to \infty \tag{2.15}$$

and since the unperturbed wavefunction describes a bound state, we conclude that α is real.

Next consider the full wavefunction and define

$$e^{G_0 - G} = P + iQ \tag{2.16}$$

where P, Q are real. Then

$$\psi = \psi_0 \, e^{G_0 - G} \sim (-i\alpha \, e^W)(P + iQ) \qquad \Phi = \operatorname{Re} \psi \sim \alpha Q \, e^W. \tag{2.17}$$

For a physical state, $\Phi(x) \to 0$ as $x \to \infty$, hence we must have $Q \to 0$ (in fact faster than e^{-W}). Since the imaginary part of $\exp(G - G_0)$ vanishes, we must have $\operatorname{Im}(G - G_0) \to 0$ as well. (Strictly speaking, $\operatorname{Im}(G - G_0) \to m\pi$, $m = $ integer; however, if this is to hold order by order in λ, then $m = 0$.) So the quantization condition is

$$\operatorname{Im} G_n(\infty) = \operatorname{Im} \int_0^\infty \mathrm{d}x \, g_n(x) = 0. \tag{2.18}$$

Written more explicitly,

$$\operatorname{Im} \int_0^\infty \frac{\mathrm{d}x}{\rho(x)} \int_0^x \mathrm{d}y \, \rho(y)[E_n - \tilde{U}_n(y)] = 0. \tag{2.19}$$

Since $\tilde{U}_n$ involves lower order quantities only, (2.19) determines E_n, which is then put into (2.10) to find g_n, completing the hierarchy. So in principle we have a method for doing the bound state perturbation order by order, using on-shell information only (i.e. the unperturbed states at other energies are not needed) and involving quadratures only.

3. The energy corrections

3.1. General form

The energy correction in (2.19) can be written as

$$E_n = \frac{\operatorname{Im} J(\tilde{U}_n)}{\operatorname{Im} J(1)} \tag{3.1}$$

where we have used the notation

$$J(S) = \int_0^\infty \frac{\mathrm{d}x}{\rho(x)} \int_0^x \mathrm{d}y \, \rho(y) S(y) \tag{3.2}$$

for any function S. In this section we shall show that $J(S)$ can be reduced to a single integral. From (2.5), (2.6) and (2.9), we have

$$\psi_0 \Phi_0' - \psi_0' \Phi_0 = i\sigma \tag{3.3}$$

or

$$\psi_0^2 \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\Phi_0}{\psi_0}\right) = i\sigma \tag{3.4}$$

which allows us to write $1/\rho = 1/\psi_0^2$ as a derivative:

$$\frac{1}{\rho} = \frac{1}{i\sigma}\frac{d}{dx}\left(\frac{\Phi_0}{\psi_0}\right). \tag{3.5}$$

Next interchange order of integration in (3.2):

$$J(S) = \int_0^\infty dy\,\rho(y)S(y)\int_y^\infty \frac{dx}{\rho(x)} \tag{3.6}$$

and perform the x-integral by using (3.5)

$$\int_y^\infty \frac{dx}{\rho(x)} = \frac{i}{\sigma}\frac{\Phi_0(y)}{\psi_0(y)} \tag{3.7}$$

since Φ_0/ψ_0 vanishes at $x \to \infty$. Therefore

$$J(S) = \frac{i}{\sigma}\int_0^\infty dy\,\rho(y)S(y)\Phi_0(y)/\psi_0(y)$$

$$= \frac{i}{\sigma}\int_0^\infty dy\,\Phi_0(y)\psi_0(y)S(y). \tag{3.8}$$

So putting this into (3.1), we have

$$E_n = N_n/D \tag{3.9}$$

where

$$N_n = \operatorname{Re}\int_0^\infty dy\,\Phi_0(y)\psi_0(y)\tilde{U}_n(y) \tag{3.10}$$

and

$$D = \int_0^\infty dy\,\Phi_0(y)^2. \tag{3.11}$$

We refer to this method of obtaining the energy shifts via (3.9)–(3.11) as the explicit ghost state method. Note that D depends only on the physical wavefunction Φ but not on Im ψ or on σ, and is just the usual normalizing integral which can be set equal to 1. On general ground, the dependence on σ must cancel in N_n. This property will be verified up to and including the third-order energy shift. The most direct way of applying the present formalism is to evaluate (3.9)–(3.11) without further manipulations. However, since N_n has an apparent σ-dependence through ψ_0 and U_n, it is necessary to verify, through a simple example, that the computed energy shift is indeed σ-independent. This we shall do for the second-order energy shift for a stretched square well in the appendix.

3.2. The first-order energy correction

For the first-order correction, $\tilde{U}_1 = U$ is purely real, so the correction reduces to

$$E_1 = \int_0^\infty dy\,\Phi_0^2(y)U(y) \tag{3.12}$$

as expected. We assume D is properly normalized to 1.

3.3. The second-order energy correction

From (3.9)-(3.11) and (2.10)-(2.12), we see that

$$E_2 = -\tfrac{1}{2}\mathrm{Re}\int_0^\infty \mathrm{d}y\, \frac{\Phi_0(y)}{\rho(y)\psi_0(y)}\, h_1^2(y). \tag{3.13}$$

On using (3.5) and integrating by part once, this becomes

$$E_2 = \frac{1}{4\sigma}\,\mathrm{Im}\int_0^\infty \mathrm{d}y\,\left(\frac{\Phi_0}{\psi_0}\right)^2 2h_1(y)h_1'(y). \tag{3.14}$$

On substituting (2.10b) for h_1, we get

$$E_2 = \frac{1}{\sigma}\,\mathrm{Im}\int_0^\infty \mathrm{d}y\, \Phi_0^2(y)F_1(y)2\int_0^y \mathrm{d}z\, F_1(z)[\Phi_0(z)+\mathrm{i}\sigma\chi_0(z)]^2. \tag{3.15}$$

Since Φ_0, χ_0 and F_1 are all real functions, on taking the imaginary part, this becomes

$$E_2 = 4\int_0^\infty \mathrm{d}y\, \Phi_0^2(y)F_1(y)\int_0^y \mathrm{d}z\, F_1(z)\Phi_0(z)\chi_0(z) \tag{3.16}$$

with

$$F_1(x) = E_1 - U(x). \tag{3.17}$$

Note that the σ-dependence has disappeared and that χ_0 is fixed by the Wronskian being equal to 1.

3.4. Connection to the Green function method

We shall now show that (3.16) is equivalent to the second order energy shift in terms of the Green function. The upper limit of the inner integral can be extended to infinity with the help of the step function ϑ and the resulting expression is then symmetrized, arriving at

$$E_2 = \int_0^\infty \int_0^\infty \mathrm{d}y\, \mathrm{d}z\, \Phi_0(y)F_1(y)\,\mathscr{G}(y, z)F_1(z)\Phi_0(z) \tag{3.18}$$

where

$$\mathscr{G}(y, z) = 2[\Phi_0(y)\chi_0(z)\vartheta(y-z) + \chi_0(y)\Phi_0(z)\vartheta(z-y)]. \tag{3.19}$$

Equation (3.19) is the usual construction of the unperturbed Green function subject to the Wronskian property in (2.5) and it can be trivially verified that

$$\mathscr{G}(y, z) = \langle y|(E_0 - H_0)^{-1}|z\rangle \equiv \langle y|\mathscr{G}|z\rangle \tag{3.20}$$

since Φ_0 and χ_0 are both eigenfunctions of H_0 with eigenvalue E_0 and according to (3.3)

$$\Phi_0'(z)\chi_0(z) - \Phi_0(z)\chi_0'(z) = 1. \tag{3.21}$$

The appearance of F_1 instead of the perturbation U in (3.18) ensures that the initial state Φ_0 is projected out of the Green function. Then the expression in (3.19) is equivalent to

$$E_2 = \langle\Phi_0| UQ\mathscr{G}QU|\Phi_0\rangle \tag{3.22}$$

where

$$Q = 1 - |\Phi_0\rangle\langle\Phi_0| \tag{3.23}$$

is the projection operator. Equation (3.23) is the usual expression for the second order energy shift.

3.5. The third-order energy correction

According to (3.9), the third order energy shift is given by

$$E_3 = -\operatorname{Re} \int_0^\infty \mathrm{d}y \frac{\Phi_0(y)\psi_0(y)}{\rho(y)^2} h_1(y)h_2(y).$$

(3.24)

The best way to remove the σ-dependence would seem to be by taking $\sigma \to 0$, but on the face of it, this integrand seems to have a second-order pole if σ is set equal to zero. However, by means of the technique used in the previous subsection through the use of (3.5), this singularity is removable by repeated integrations by parts. Upon doing so, the σ-dependent quantities are found to vanish. The procedure, though tedious, is straightforward. We shall only give the final result here:

$$E_3 = -8 \int_0^\infty \mathrm{d}x \, \Phi_0(x)^2 F_1(x)[J_1(x) + J_2(x)]$$

(3.25)

where

$$J_1(x) = \int_0^x \mathrm{d}y \, \Phi_0^2(y)F_1(y) \int_0^y \mathrm{d}z \, \chi_0^2(z)F_1(z)$$

(3.26)

and

$$J_2(x) = 2 \int_0^x \mathrm{d}y \, \Phi_0(y)\chi_0(y)F_1(y) \int_0^y \mathrm{d}z \, \Phi_0(z)\chi_0(z)F_1(z).$$

(3.27)

In this derivation, we have utilized the property that

$$\int_0^\infty \int_0^\infty \mathrm{d}y \, \mathrm{d}x \, \Phi_0(y)F_1(y)\mathscr{G}(y,x)\Phi_0(x) = 0.$$

(3.28)

By a direct substitution of (3.19), (3.20) and (3.21), we verify that the usual expression for the third-order energy shift

$$E_3 = \langle \Phi_0 | UQ\mathscr{G}QUQ\mathscr{G}QU | \Phi_0 \rangle$$

(3.29)

written here for the simple case $E_i = 0$ without loss of generality is identical to the expression for E_3 given in (3.25). We refer to this method of obtaining the energy shifts via (3.16) and (3.25) as the ghost state retention method.

3.6. Implication

The fact that the physical entities (the energy corrections) are independent of σ indicates that one can even set σ zero. This implies that for excited states, the singularities at the nodal points are removable. However, for an arbitrary situation where the analytic form of the wavefunction is unavailable, one may not be able to perform integration by parts to remove these apparent singularities. In this case, one is bound to encounter the logarithmic singularities at the nodes if the wavefunction is taken to be that of the physical state alone. By mixing in the ghost state, the zeros are bypassed, by as much as is convenient in a numerical calculation.

In the next section, we shall use the quartic x^4 anharmonic perturbation on the third excited state of the harmonic oscillator and obtain the second-order energy shift via (3.13) with σ equal to zero (the *ad hoc* straightforward logarithmic perturbation method) and via (3.16) (the ghost state retention method). The answer is identical to

that obtained with the sum over intermediate states method. While the ghost state retention method gives an unambiguous answer, we shall justify the *ad hoc* prescription of the usual logarithmic perturbation theory without any modification.

4. An example: the quartic anharmonic oscillator

We consider here the perturbation λx^4 to the Hamiltonian $H_0 = \frac{1}{2}(p^2 + x^2)$, and concern ourselves with the third excited state, $n = 3$, which may be regarded as the first excited state of the half-line problem satisfying (2.3*a*). By the usual Rayleigh–Schrödinger perturbation theory, one finds

$$E = \frac{7}{2} + \frac{75}{4}\lambda - \frac{1575}{8}\lambda^2 + \ldots . \tag{4.1}$$

4.1. The second-order energy shift via the fundamental logarithmic perturbation method

The unperturbed state under consideration is

$$\Phi_0(x) = \frac{\sqrt{6}}{\pi^{1/4}} \left[-\frac{2}{3}x^3 + x \right] e^{-x^2/2}. \tag{4.2}$$

According to (3.17), we have

$$F_1(x) = \frac{\lambda}{4}[75 - 4x^4]. \tag{4.3}$$

Putting this into (2.10*b*), with $\sigma = 0$, then gives

$$h_1(x) = \lambda x^3 P(x) \, e^{-x^2}/(3\sqrt{\pi}) \tag{4.4}$$

where

$$P(x) = 8x^6 + 12x^4 - 90x^2 + 225. \tag{4.5}$$

When this is inserted into (3.13), with $\sigma = 0$, we find

$$E_2 = \frac{-\lambda^2}{48\sqrt{\pi}} \int_0^\infty dx \, e^{-x^2}[x^2 P(x)]^2/(x^2 - 3/2)^2. \tag{4.6}$$

This expression is ill-defined on account of the pole at the node of Φ_0 at $x = x_1 = \sqrt{\frac{3}{2}}$. However, if we adopt the *ad hoc* prescription of treating such singular factors as distributions and integrating by parts:

$$\int_0^\infty dx f(x)(x - x_i)^{-n} = \int_0^\infty dx f(x) \frac{(-1)^{n-1}}{(n-1)!} \frac{d^n}{dx^n} \ln|x - x_i|$$

$$= -\frac{1}{(n-1)!} \int_0^\infty dx \frac{d^n f(x)}{dx^n} \ln|x - x_i| \tag{4.7}$$

then (4.6) becomes non-singular and can be evaluated. Note that the polynomial in the integrand in (4.6) vanishes rapidly at $x = 0$ (in fact like x^4) so that no surface terms are introduced upon integration by parts. The result of evaluating E_2 by this prescription is in agreement with (4.1).

In section 5 we shall show that such a prescription is indeed appropriate and also give an equivalent and sometimes more convenient method of evaluating integrals such as (4.7).

4.2. The second-order energy correction via the ghost state retention method

The ghost state that satisfies the normalization condition (2.5) is

$$\chi_0(x) = \frac{\pi^{1/4}}{\sqrt{6}} \left[(2x^3 - 3x) \, e^{-x^2/2} \eta(x) - (x^2 - 1) \, e^{x^2/2} \right] \tag{4.8}$$

where

$$\eta(x) \equiv \int_0^x e^{t^2} \, dt. \tag{4.8a}$$

Note that the ghost state of energy $n + \frac{1}{2}$ can be obtained from the ghost state of energy $\frac{1}{2}$ by using the raising operator in the usual way. Then the second order energy shift E_2 according to (3.16) is of the form

$$\text{constant} \times \int_0^\infty dx \, e^{-x^2} Q(x) [Y_1(x) + Y_2(x)] \tag{4.9}$$

where $Q(x)$ and $Y_2(x)$ are polynomials, and

$$Y_1(x) = -\int_0^x dy \, e^{-y^2} Q(y) \eta(y) \tag{4.10}$$

for the same Q. It turns out that Q can be written as

$$\frac{d}{dy} [e^{-y^2} R(y)] = e^{-y^2} Q(y) \tag{4.11}$$

where R is another polynomial; in fact

$$R(y) = 8y^9 + 12y^7 - 90y^5 + 225y^3. \tag{4.12}$$

Using (4.11) in (4.10) and integrating by parts

$$Y_1(x) = -e^{-x^2} R(x) \eta(x) + \int_0^x dy \, R(y). \tag{4.13}$$

Now Y_2, and the second term in Y_1, when put into (4.9), is of the form

$$\int_0^\infty dx \, e^{-x^2} \times (\text{polynomial}) \tag{4.14}$$

and is readily evaluated. The first term in Y_1 contributes

$$\int_0^\infty dx \frac{d}{dx} [e^{-x^2} R(x)][-e^{-x^2} R(x) \eta(x)]$$

$$= -\tfrac{1}{2} \int_0^\infty dx \frac{d}{dx} [e^{-x^2} R(x)]^2 \eta(x)$$

$$= +\tfrac{1}{2} \int_0^\infty dx [e^{-x^2} R(x)]^2 e^{x^2} \tag{4.15}$$

which is again of the form (4.14), and hence readily evaluated. Upon carrying out the arithmetic, one finds that E_2 agrees with the second-order term in (4.1).

It is stressed that there is no ambiguity and no room for *ad hoc* prescriptions in this evaluation.

5. Justification of *ad hoc* prescription

We have seen that the ghost-state method gives an ambiguous result, while the straightforward perturbation method (i.e. setting $\sigma = 0$ from the start) contains an ambiguity which, upon being specified by the *ad hoc* prescription of integrating by parts, does yield the correct answer. In this section, we sketch a justification of this prescription. We only use the properties of the wavefunctions of the physical and ghost states near the zeros of the physical state, in accordance with the Wronskian condition (2.5).

Start with the ghost-state method and consider the possibility of taking $\sigma \to 0$. The only trouble occurs near the nodes x_i of $\Phi_0(x)$, in integrals of the form

$$\text{Re} \int dx f(x)/\psi_0(x)^n. \tag{5.1}$$

Except for the factors of ψ_0 in the denominator, everywhere else we may set $\sigma = 0$, in which case $f(x)$ is real. Now, near x_i, Φ_0 has a first-order zero, say

$$\Phi_0(x) = \alpha(x - x_i) + \ldots \tag{5.2}$$

and by (2.5) we see that

$$\chi_0(x) = \frac{1}{\alpha} + \beta(x - x_i) + \ldots \tag{5.3}$$

from which it is easy to see that for $\sigma \to 0$, there is a root of ψ_0 at the position

$$\tilde{x}_i = x_i - i\sigma/\alpha^2 + O(\sigma^2) \tag{5.4}$$

and the singular (hence ambiguous when $\sigma = 0$) part of (5.1) is of the form

$$\text{Re} \int dx f(x)(x - \tilde{x}_i)^{-n} \tag{5.5}$$

and the same manipulations as in (4.7) can be applied. However, in this case, since $\tilde{x}_i$ is off the real axis, these manipulations are not merely formal, but fully justified. After all the integrations by parts have been performed, we then take $\sigma \to 0$, which simply turns $\tilde{x}_i$ into x_i, giving the final form in (4.7). We refer to this as the limiting ghost state method.

An alternative method is to differentiate with respect to the parameter $\tilde{x}_i$:

$$\text{Re} \int dx f(x)(x - \tilde{x}_i)^{-n} = \frac{1}{(n-1)!} \left(\frac{d}{d\tilde{x}_i}\right)^{n-1} \text{Re} \int dx f(x)(x - \tilde{x}_i)^{-1}$$

$$= \frac{1}{(n-1)!} \left(\frac{d}{d\tilde{x}_i}\right)^{n-1} P \int dx f(x)(x - \tilde{x}_i)^{-1} \tag{5.6}$$

where P denotes principal value. This method is obviously equivalent to (4.7) and is in fact more convenient because there is no need to differentiate f, and principal-value integrals are often tabulated.

6. Concluding remarks

We have introduced a method by which the singularities in the logarithmic perturbation theory for excited bound states can be bypassed. This method involves mixing the

ghost-state solution with the physical state solution. We have shown explicitly up to and including the third-order energy shift that the physical entities are independent of the amount of mixing of the ghost state and have demonstrated the equivalence with the usual Green function method. The fact that the physical entities are independent of the mixing of the ghost state implies that singularities encountered in the straightforward logarithmic perturbation theory for excited bound states must be removable singularities, and are indeed removed by the *ad hoc* prescription of integration by parts. The mixing of the ghost state moves these singularities off the real axis, and provides a justification of such manoeuvres of integration by parts. The limit of zero mixing coefficient is well defined and the formal procedures reduces to the *ad hoc* procedure. We have demonstrated this explicitly for the third excited state of the harmonic oscillator with the λx^4 perturbation. However, in a situation, such as a numerical calculation, where the procedure to remove the singularities is impractical to carry out, our method provides a convenient way out. We emphasize that we retain all the advantages of ordinarily logarithmic perturbation theory: all higher-order corrections are obtainable in a hierarchical scheme from a knowledge of the unperturbed solution alone.

As another example, we have also successfully applied the *ad hoc* procedure to the 2S state of the hydrogen atom in a rescaled Coulomb potential $-(1+\lambda)e^2/r$ where λ is a small parameter. The calculation is straightforward and the answer agrees with the exact calculation.

There are many variants of the logarithmic perturbation method, and we briefly summarize their differences and relationship with each other. (1) There is the original, straightforward, use of the logarithmic perturbation theory, derived for the ground state, but logically invalid for excited states on account of the nodal problem. Nevertheless, with an implicit *ad hoc* prescription, it somehow seems to work for excited states as well, at least for second order. This is referred to as the fundamental logarithmic perturbation method. (2) One way to cure the nodal problem is to factor out the zeros. This is referred to as the node factorization method, as discussed in detail earlier in [4]. Within the ghost-state method formulated in section 3 of this paper, there are several possibilities. (3) We can simply use the formulas as derived in section 3.1, which contains σ explicitly, to evaluate the energy corrections numerically. This is referred to as the explicit ghost-state method. In appendix A, we show, via an example, that the results are indeed σ-independent. (4) Alternatively, we can go through a series of algebraic manipulations, as shown in sections 3.3 and 3.5, to obtain results from which σ disappears completely, but in which the ghost state appears. This is referred to as the ghost-state retention method. (5) Alternatively, we can simply take the limit $\sigma \to 0$, and in section 5 we show that this limit justifies the use of the fundamental method (1) for excited bound states as we have demonstrated in section 4.1. This is referred to as the limiting ghost-state method. Most of these variants are illustrated via examples.

Appendix. An explicit demonstration of ghost state mixing independence for the energy shifts

In this appendix, we choose a simple example to show that the second order energy shift computed numerically according to (3.9)–(3.11) (the explicit ghost-state method) is indeed independent of the amount of ghost-state mixing in the wavefunction. To do so, we consider the second excited state of the stretched square well, defined by the unperturbed potential.

$$U(x) = \begin{cases} V_0 & 0 \leqslant x \leqslant b \\ 0 & \text{otherwise} \end{cases} \tag{A1}$$

and the exact potential

$$U(x) + \lambda V(x) = \begin{cases} V_0 & 0 \leqslant x \leqslant b+d \\ 0 & \text{otherwise} \end{cases} \tag{A2}$$

where as an example, we choose the parameter values

$$V_0 = -100 \qquad b = 1 \qquad d = 0.1. \tag{A3}$$

From (3.10) and (3.11), the second-order energy corrections can be written as the sum of the following three terms:

$$I_1 = -2 \int_0^\infty dx \frac{\Phi_0(x)^4 - 3\sigma^2\Phi_0(x)^2\chi_0(x)^2}{[\Phi_0(x)^2 + \sigma^2\chi_0(x)^2]^3} \left\{ \int_0^x dy\, F_1(y)[\Phi_0(y)^2 - \sigma^2\chi_0(y)^2] \right\}^2 \tag{A4}$$

$$I_2 = 2 \int_0^\infty dx \frac{\Phi_0(x)^4 - 3\sigma^2\Phi_0(x)^2\chi_0(x)^2}{[\Phi_0(x)^2 + \sigma^2\chi_0(x)^2]^3} \left[\int_0^x dy\, 2\sigma F_1(y)\Phi_0(y)\chi_0(y) \right]^2 \tag{A5}$$

$$I_3 = 2 \int_0^\infty dx \frac{2\Phi_0(x)[\sigma^3\chi_0(x)^3 - 3\sigma\chi_0(x)\Phi_0(x)^2]}{[\Phi_0(x)^2 + \sigma^2\chi_0(x)^2]^3} \int_0^x dy\, F_1(y)[\Phi_0(y)^2 - \sigma^2\chi_0(y)]$$

$$\times \int_0^x dz\, 2\sigma F_1(z)\Phi_0(z)\chi_0(z) \tag{A6}$$

where the unperturbed physical wavefunction ψ_0 and the corresponding ghost state χ_0 are readily written down and we have assumed that ψ_0 is normalized so that D in (3.11) is unity. We have evaluated I_1, I_2 and I_3 numerically for various values of σ with the results shown in table 1. It is seen that although each of these depends on σ, their sum is independent of σ and indeed agrees well with the exact value -1.70845.

Table 1. Values of the integrals I_1, I_2 and I_3 for various σ to demonstrate independence of the amount of ghost state mixing. Data refer to the second-order energy shift of the second excited state of the stretched square well.

σ	I_1	I_2	I_3	Sum
0.02	−1.081 6499	−1.300 2616	0.673 4608	−1.708 4507
0.05	0.105 7666	−1.347 2726	−0.466 9446	−1.708 4506
0.1	0.618 2073	−0.727 7554	−1.598 9026	−1.708 4507
0.2	0.526 9681	−0.193 7130	−2.041 7057	−1.708 4506
0.5	0.393 6475	0.035 8119	−2.137 9101	−1.708 4507
1.0	0.371 7098	0.049 5207	−2.129 6812	−1.708 4507
2.0	0.367 2634	0.034 8073	−2.110 5214	−1.708 4507
5.0	0.366 3202	0.016 7103	−2.091 4812	−1.708 4507
10.0	0.366 2163	0.008 8570	−2.083 5241	−1.708 4507

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