

# A New Approach to Solve the Low-lying States of the Schroedinger Equation

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We review a new iterative procedure to solve the low-lying states of the Schroedinger equation, done in collaboration with Richard Friedberg. For the groundstate energy, the  $n$ th order iterative energy is bounded by a finite limit, independent of  $n$ ; thereby it avoids some of the inherent difficulties faced by the usual perturbative series expansions. For a fairly large class of problems, this new procedure can be proved to give convergent iterative solutions. These convergent solutions include the long standing difficult problem of a quartic potential with either symmetric or asymmetric minima.

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**KEY WORDS:** Low-lying states of Schroedinger equation; convergent iterative solution; electrostatic analog; hierarchy theorem.

## 1. IMPORTANCE OF LOW-LYING STATES

It is a common belief that most of natural phenomena should be described by solutions of the Schroedinger equation. Take the non-relativistic Schroedinger equation of a system of charged particles with Coulomb interactions. In principle, this single  $N$ -dimensional second order linear partial differential equation contains in its solutions all information about many disciplines: atomic and molecular physics (except for small relativistic corrections), condensed matter physics, chemistry and biology. Furthermore, for most of these applications we need only knowledge about its low-lying states. For these low-lying states, actually we do have very good information about their wave functions when the Coulomb interaction is strong; i.e., when the wave amplitude is large. How come that we still have great

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difficulties in solving these equations? Quite often, the challenge lies in how to handle the large number of configurations when the interaction is weak.

In quantum chromodynamics (QCD) and quantum electrodynamics (QED) the tasks are even more difficult since we do not have any exact solution. Besides the very promising lattice and other numerical calculations, we rely mostly on perturbative expansions. Yet, such expansion often leads to a divergent series with zero radius of convergence, as exemplified by the perturbative calculation of the gyromagnetic ratio  $g$  of the muon (1-3):

$$\begin{aligned} \frac{1}{2}(g-2)_\mu &= \frac{1}{2} \frac{\alpha}{\pi} + 0.765857376 \left(\frac{\alpha}{\pi}\right)^2 \\ &+ 24.05050898 \left(\frac{\alpha}{\pi}\right)^3 + 131.0 \left(\frac{\alpha}{\pi}\right)^4 \\ &+ 677(40) \left(\frac{\alpha}{\pi}\right)^5 + \dots, \end{aligned} \quad (1.1)$$

where  $\alpha$  is the fine-structure constant. The coefficients are all positive, and each successive one becomes larger and larger. There are good reasons (4) to believe that the vacuum state of QED would be unstable against pair creations if  $\alpha$  could be analytically continued to the negative region. Thus, the difficulty of perturbative series seems to be again closely related to our inability to solve the low-lying states of the corresponding Schroedinger equation. In QCD, because of the existence of instanton configurations, similar serious problems also exist for its vacuum and other low-lying states.

This situation may be illustrated by the following one-dimensional problem with a quartic potential of degenerate minima. The Schroedinger equation can be written as

$$(T + V - E)\psi = 0, \quad (1.2)$$

where  $T = -\frac{1}{2} \frac{d^2}{dx^2}$  and

$$V(x) = \frac{1}{2} g^2 (x^2 - a^2)^2. \quad (1.3)$$

An alternative form of the same problem may be obtained by setting  $q \equiv \sqrt{2ga}(a-x)$ , so that the Hamiltonian becomes

$$H = T + V \equiv 2ga\mathcal{H} \quad (1.4)$$

with

$$\mathcal{H} = -\frac{1}{2} \frac{d^2}{dq^2} + \frac{1}{2} q^2 (1 - e^{-q})^2, \tag{1.5}$$

in which  $\mathcal{H}$ ,  $q$  and  $e = 1/\sqrt{8ga^3}$  are all dimensionless. The perturbative expression of the groundstate energy  $E$  is (5-14)

$$E = ga - \frac{1}{4a^2} - \frac{9}{64} \frac{1}{ga^5} - \frac{89}{512} \frac{1}{g^2 a^8} - O\left(\frac{1}{g^3 a^{11}}\right), \tag{1.6}$$

or, in terms of the dimensionless coupling  $e^2$

$$E = 2ga \left[ \frac{1}{2} - e^2 - \frac{9}{2} e^4 - \frac{89}{2} e^6 - \dots \right], \tag{1.7}$$

which has a similar characteristics as the  $(g - 2)$  expansion (1.1).

In this one-dimensional case, from (1.5), one sees that for  $e^2$  negative,  $\mathcal{H}$  has no groundstate; this explains why the power series (1.7) is divergent. For  $e^2 = 1/8ga^3$  positive, it is also possible to trace the origin of the difficulty. The corresponding perturbative series of the groundstate wave function  $\psi(x)$  may be written as

$$\psi(x) = e^{-gS_0 - S_1 - g^{-1}S_2 - g^{-2}S_3 - \dots} \tag{1.8}$$

Since the potential  $V(x)$  has two degenerate minima at  $x = \pm a$ , there are two different expansions depending on the normalization condition:

$$\psi(a) = 1, \quad \text{or} \quad \psi(-a) = 1. \tag{1.9}$$

In either case, the perturbative series is divergent for any  $g$ . However, for  $g$  large, the wave function  $\psi(x)$  can be approximately described by the first two terms of these expansions. For  $x > 0$ , using the normalization  $\psi(a) = 1$ , we find

$$e^{-gS_0 - S_1} = \frac{2a}{a+x} e^{-\frac{g}{3}(a-x)^2(2a+x)}, \tag{1.10}$$

and for  $x < 0$  with  $\psi(-a) = 1$ ,

$$e^{-gS_0 - S_1} = \frac{2a}{a-x} e^{-\frac{g}{3}(a+x)^2(2a-x)}. \tag{1.11}$$

Unlike  $\psi(x)$ , neither expression has a zero derivative at  $x=0$ . Furthermore, each carries a spurious pole-term, at  $x=-a$  for (1.10) and  $x=a$  for (1.11). In addition, if one stays with the perturbative series (1.8), each successive higher order expansion accentuates further these spurious pole terms. This suggests that we must not follow the high order perturbative expressions, especially in the region  $x$  near 0, when  $\psi(x)$  is exponentially small.

In all these problems, it is not difficult to construct a trial function  $\phi$  such that

$$\phi \approx \psi \quad \text{when } \psi \text{ is large,} \quad (1.12)$$

and with the correct symmetry properties of  $\psi$  (e.g.,  $\phi(x) = \phi(-x)$  for the quartic potential problem (1.2)–(1.3)). The question is how to devise a convergent procedure that can lead from the trial function  $\phi$  to the correct  $\psi$ .

In the following we will discuss such a method by first following the approach developed in a recent series papers by Friedberg *et al.*<sup>(15–19)</sup>. Next, we generalize several of their results proved for one-dimensional problems to  $N$ -dimension. In particular, the extension of the hierarchy theorem to a radially symmetric potential in  $N$ -dimension discussed in Section 4 and its proof given in Appendix B are both new results. In addition, Appendix C contains a new comparison between this iterative approach and the usual perturbative expansion.

## 2. THE NEW METHOD

As examples of the types of Schroedinger equations that we are interested, consider the bosonic component of QED or QCD in the axial gauge, or a system of nonrelativistic particles. In either of these cases the kinetic energy  $T$  is a quadratic function of momentum operators. Through a linear transformation of the relevant coordinate variables, the Hamiltonian  $H$  can be written as

$$H = T + V(q), \quad (2.1)$$

where

$$q = (q_1, q_2, \dots, q_N) \quad (2.2)$$

and

$$T = -\frac{1}{2} \sum_{i=1}^N \partial^2 / \partial q_i^2 = -\frac{1}{2} \nabla^2 \quad (2.3)$$

with  $N = \infty$  in the case of a field theory. Let  $\psi(q)$  be the groundstate determined by

$$(H - E)\psi = 0. \quad (2.4)$$

To derive  $\psi(q)$ , we proceed as follows (15–19):

1. Construct a good trial function  $\phi(q)$ , so that

$$\phi(q) \approx \psi(q) \quad (2.5)$$

in regions when  $\psi(q)$  is expected to be large. An example of how to construct such a trial function is given in Appendix A.

2. Construct  $U(q) - E_0$  by differentiating  $\phi(q)$ :

$$U(q) - E_0 \equiv \left( \frac{1}{2} \nabla^2 \phi \right) / \phi. \quad (2.6)$$

Define

$$H_0 = -\frac{1}{2} \nabla^2 + U(q). \quad (2.7)$$

We have

$$(H_0 - E_0)\phi(q) = 0. \quad (2.8)$$

Introduce the differences  $h$  and  $\mathcal{E}$  by

$$H_0 - H = U(q) - V(q) \equiv h(q) \quad (2.9)$$

and

$$E_0 - E \equiv \mathcal{E}. \quad (2.10)$$

The original Schroedinger equation (2.4) can be written as

$$(H_0 - E_0)\psi(q) = (h - \mathcal{E})\psi(q). \quad (2.11)$$

We assume that the trial function is well chosen so that  $h(q)$  is well-behaved at  $\infty$ . From the definitions (2.9) and (2.10), we see that since

$$h(q) - \mathcal{E} = [U(q) - E_0] - [V(q) - E] \quad (2.12)$$

depends only on the difference  $[U(q) - E_0]$ , we can choose the constant  $E_0$  by requiring that  $q = \infty$ ,

$$h(\infty) = 0. \quad (2.13)$$

For the discussions of the groundstate, we take both

$$\psi(q) \text{ and } \phi(q) \text{ to be real and positive.} \quad (2.14)$$

Multiplying (2.11) by  $\phi(q)$  and (2.8) by  $\psi(q)$ , then taking their difference, we have

$$-\frac{1}{2} \nabla \cdot (\phi \nabla \psi - \psi \nabla \phi) = (h - \mathcal{E}) \phi \psi. \quad (2.15)$$

The integration of (2.15) over all space gives  $\int (h - \mathcal{E}) \phi \psi d^N q = 0$ ; therefore,

$$\mathcal{E} = \frac{\int h \phi \psi d^N q}{\int \phi \psi d^N q}. \quad (2.16)$$

It is convenient to introduce

$$f(q) = \psi(q) / \phi(q); \quad (2.17)$$

(2.16) becomes then

$$\mathcal{E} = \frac{\int h(q) \phi^2(q) f(q) d^N q}{\int \phi^2(q) f(q) d^N q}. \quad (2.18)$$

3. We propose to solve the Schroedinger equation (2.11) by an iterative process, defined by

$$(H_0 - E_0) \psi_n(q) = (h(q) - \mathcal{E}_n) \psi_{n-1}(q) \quad (2.19)$$

with  $n = 1, 2, \dots$  and for  $n = 0$ ,

$$\psi_0(q) = \phi(q). \quad (2.20)$$

Multiplying (2.19) by  $\phi(q)$  and (2.8) by  $\psi_n(q)$ , then taking their difference, we derive

$$-\frac{1}{2} \nabla \cdot (\phi \nabla \psi_n - \psi_n \nabla \phi) = (h - \mathcal{E}_n) \phi \psi_{n-1}. \quad (2.21)$$

Analogous to (2.16), we have

$$\mathcal{E}_n = \int h \phi \psi_{n-1} d^N q \bigg/ \int \phi \psi_{n-1} d^N q. \tag{2.22}$$

Note that in each step of the iteration from  $n - 1$  to  $n$ , for any particular solution  $\psi_n^0(q)$  that satisfies (2.19), so is

$$\psi_n(q) = \psi_n^0(q) + c_n \phi(q) \tag{2.23}$$

also a solution where  $c_n$  is an arbitrary constant. Since  $\phi(q)$  is positive in accordance with (2.14), we can choose  $c_n$  so that

$$\psi_n(q) \text{ is positive everywhere.} \tag{2.24}$$

It is clear that (2.24) can be realized in the  $q$ -space within any finite domain, however large, because of (2.13), the same conclusion (2.14) also holds for the entire  $q$ -space, including infinity. (The same property can also be established by using the electrostatic analog, which will be discussed in the next section.)

Define

$$f_n(q) = \psi_n(q) / \phi(q) \tag{2.25}$$

and therefore (2.22) becomes

$$\mathcal{E}_n = \int h \phi^2 f_{n-1} d^N q \bigg/ \int \phi^2 f_{n-1} d^N q. \tag{2.26}$$

From (2.24), we have

$$f_n(q) \text{ positive.} \tag{2.27}$$

As we shall see, a particularly convenient choice of the constant  $c_n$  is to set the minimum of  $f_n(q)$  to be 1 and therefore

$$f_n(q) \geq 1. \tag{2.28}$$

From (2.26) and (2.27), it follows that  $\mathcal{E}_n$  is bounded if  $h(q)$  is bounded. Therefore, as  $n \rightarrow \infty$ ,  $\lim \mathcal{E}_n$  cannot be  $\infty$ . This avoids the type of divergence difficulties that appears in the example (1.7). It is therefore reasonable to expect that  $\lim_{n \rightarrow \infty} \mathcal{E}_n$  should converge to the correct  $\mathcal{E}$ , at least

when  $h$  is small. As we shall see, for a fairly large class of problems, including the quartic potential (1.3), the convergence of  $\mathcal{E}_n$  turns out to be independent of the magnitude of  $h(q)$ , provided that it is finite and satisfies some general conditions.

In this paper, we concentrate on the groundstate. Extensions to some low-lying states can be found in ref. 17.

### 3. AN ELECTROSTATIC ANALOG

In terms of the ratio  $f_n = \psi_n/\phi$  introduced in (2.25), the  $n$ th order iterative equation (2.21) can be written as

$$-\frac{1}{2}\nabla \cdot (\phi^2 \nabla f_n) = \sigma_n(q), \quad (3.1)$$

where

$$\sigma_n(q) \equiv (h(q) - \mathcal{E}_n)\phi^2(q) f_{n-1}(q) \quad (3.2)$$

and when  $n=0$ ,

$$f_0(q) = 1 \quad (3.3)$$

in accordance with (2.20). Assuming that  $\psi_{n-1}(q)$  has already been solved, we can determine  $\mathcal{E}_n$  through (2.22). Therefore,  $\sigma_n(q)$  is a known function.

Consider a dielectric medium with a  $q$ -dependent dielectric constant, given by

$$\kappa(q) \equiv \phi^2(q). \quad (3.4)$$

Interpret  $\sigma_n(q)$  as an external electrostatic charge distribution,  $\frac{1}{2}f_n$  the electrostatic potential,  $-\frac{1}{2}\nabla f_n$  the electrostatic field and

$$D_n \equiv -\frac{1}{2}\kappa \nabla f_n \quad (3.5)$$

the corresponding displacement vector field. Thus (3.1) becomes

$$\nabla \cdot D_n = \sigma_n, \quad (3.6)$$

the Maxwell equation for this electrostatic analog problem.



At infinity,  $\phi(\infty) = 0$ . In accordance with (3.4)–(3.5), we also have  $D_n(\infty) = 0$ . Hence the integration of (3.6) leads to the total external electrostatic charge to be also zero; i.e.,

$$\int \sigma_n(q) d^N q = 0 \tag{3.7}$$

which is the same result given by (2.26) for the determination of  $\mathcal{E}_n$ . Because the dielectric constant  $\kappa(q)$  in this analog problem is zero at  $q = \infty$ , the dielectric media becomes a perfect dia-electric at  $\infty$ . Thus, the equation of zero total charge, given by (3.7), may serve as a much simplified model of charge confinement, analogous to color confinement in quantum chromodynamics.

We note that (3.1) can also be derived from a minimal principle by defining

$$I(f_n(q)) \equiv \int \left\{ \frac{1}{4} \kappa (\nabla f_n)^2 - \sigma_n f_n \right\} d^N q. \tag{3.8}$$

Because of (3.7), the functional  $I(f_n(q))$  is invariant under

$$f_n(q) \rightarrow f_n(q) + \text{constant}. \tag{3.9}$$

Since the quadratic part of  $I(f_n(q))$  is the integral of the positive definite  $\frac{1}{4} \kappa (\nabla f_n)^2$ , the curvature of  $I(f_n(q))$  in the functional space  $f_n(q)$  is always positive. Hence,  $I(f_n(q))$  has a minimum, and that minimum determines a unique electrostatic field  $-\frac{1}{2} \nabla f_n$ , as we shall see. To establish the uniqueness, let us assume two different  $\nabla f_n$ , both satisfy (3.1), with the same  $\kappa = \phi^2$  and the same  $\sigma_n$ ; their difference would then satisfy (3.1) with a zero external charge distribution. For  $\sigma_n = 0$ , the minimum of  $I(f_n(q))$  is clearly zero with the corresponding  $\nabla f_n = 0$ . To derive  $f_n(q)$  from  $\nabla f_n$ , there remains an additive constant at each iteration, as already noted in (2.23). As we shall discuss in the next section, this arbitrariness allows us the freedom to derive different types of convergent series.

We note that in this electrostatic analog, the problem depends only on two input-functions:  $\phi^2(q)$  and the product

$$h(q) \phi^2(q). \tag{3.10}$$

The original potential  $V(q)$  no longer appears explicitly. Consider, e.g., a system of particles with electric charges. For configurations when the

Coulomb energy  $V(q)$  is attractive and near its singularity, we have good knowledge about the wave amplitude  $\psi(q)$ , which is large but regular. The same should be true for a good trial function  $\phi(q)$ . In accordance with (1.12), we expect

$$h(q) \text{ small, when } \psi \text{ is large.} \tag{3.11}$$

For configurations when  $\psi$  is small, so should be  $\phi$ . Thus, a good trial function  $\phi$  would result in a small  $h\phi^2$  everywhere even though  $h$  may not.

When  $N = 1$ , we may denote the coordinate (2.2) by a single  $x$ . Correspondingly (3.5) and (3.6) become

$$D_n = -\frac{1}{2}\kappa \frac{df_n}{dx} \tag{3.12}$$

and

$$\frac{dD_n}{dx} = \sigma_n(x). \tag{3.13}$$

Since  $D_n(\infty) = 0$ , we have

$$D_n(x) = -\int_x^\infty \sigma_n(z) dz \tag{3.14}$$

and therefore

$$f_n(x) = f_n(\infty) - 2 \int_x^\infty \phi^{-2}(y) dy \int_y^\infty \sigma_n(z) dz \tag{3.15}$$

with

$$\sigma_n(x) = (h(x) - \mathcal{E}_n)\phi^2(x)f_{n-1}(x), \tag{3.16}$$

which satisfies

$$\int_{-\infty}^\infty \sigma_n(x) dx = 0. \tag{3.17}$$

Therefore,

$$D_n(-\infty) = D_n(\infty) = 0 \tag{3.18}$$

and

$$f_n(\infty) - f_n(-\infty) = 2 \int_{-\infty}^{\infty} \phi^{-2}(y) dy \int_y^{\infty} \sigma_n(z) dz. \tag{3.19}$$

When  $N > 1$ , for radially symmetric problems we have

$$h = h(r), \quad \phi^2 = \kappa(r) \tag{3.20}$$

where

$$r^2 = q_1^2 + q_2^2 + \dots + q_N^2. \tag{3.21}$$

Likewise  $\psi$ ,  $\psi_n$  and  $\sigma_n$  are all functions of  $r$  only. The radial component of  $D_n$  is

$$(D_n)_r = -\frac{1}{2} \kappa(r) \frac{df_n(r)}{dr}. \tag{3.22}$$

Correspondingly, (3.6) becomes

$$\frac{1}{r^{N-1}} \frac{d}{dr} \left( r^{N-1} (D_n)_r \right) = \sigma_n(r) \tag{3.23}$$

with

$$\sigma_n(r) = (h(r) - \mathcal{E}_n) \phi^2(r) f_{n-1}(r).$$

Hence,

$$(D_n)_r = -\frac{1}{r^{N-1}} \int_r^{\infty} z^{N-1} \sigma_n(z) dz \tag{3.24}$$

and on account of (3.22),

$$f_n(r) = f_n(\infty) - \int_r^{\infty} \frac{2 dy}{y^{N-1} \phi^2(y)} \int_y^{\infty} z^{N-1} \sigma_n(z) dz. \tag{3.25}$$

Assuming as  $r \rightarrow \infty$ ,

$$\phi^2(r) \rightarrow a e^{-br^l} \tag{3.26}$$

with  $a$ ,  $b$  and  $l$  all positive constants. We assume

$$l > 2. \quad (3.27)$$

In accordance with (3.16), as  $r \rightarrow \infty$

$$\sigma_n(r) \rightarrow c e^{-br^l}, \quad (3.28)$$

where

$$c = (h(\infty) - \mathcal{E}_n) a f_{n-1}(\infty). \quad (3.29)$$

By partial integrations, we see that as  $r \rightarrow \infty$ ,

$$f_n(r) \rightarrow f_n(\infty) - \frac{2}{b} \frac{(h(\infty) - \mathcal{E}_n) f_{n-1}(\infty)}{l(l-2)r^{l-2}} \left[ 1 + O\left(\frac{1}{br^l}\right) \right]. \quad (3.30)$$

When the dimension  $N = 1$ , the same expression applies, with  $r$  replaced by  $x$ .

Because of (3.7), in the  $N > 1$  radially symmetric case we have

$$\int_0^\infty r^{N-1} \sigma_n(r) dr = 0, \quad (3.31)$$

therefore (3.25) is identical to

$$f_n(r) = f_n(0) - \int_0^r \frac{2 dy}{y^{N-1} \phi^2(y)} \int_0^y z^{N-1} \sigma_n(z) dz. \quad (3.32)$$

When  $N = 1$  and  $V(x)$  is an even function of  $x$ , (3.32) applies with the replacement of  $r$  by  $x$ ; if  $V(x)$  is not an even function then we have, from (3.15) and (3.19),

$$f_n(x) = f_n(-\infty) - 2 \int_{-\infty}^x \phi^{-2}(y) dy \int_{-\infty}^y \sigma_n(z) dz. \quad (3.33)$$

For an arbitrary  $N > 1$  dimensional radially non-symmetric problem, the general solution of the electrostatic analog problem can no longer be reduced to simple quadratures. Thus, numerical analysis may become important. In that case, the minimal principle using the functional  $I(f(q))$  given by (3.8) may be of some practical use.

#### 4. HIERARCHY THEOREM

In this section we restrict our discussions to either (i) the  $N$ -dimensional radially symmetric case in which the functions  $V$  in (2.1) and  $h$  in (2.9) are

$$V = V(r) \quad \text{and} \quad h = h(r) \quad (4.1)$$

where  $r^2 = q_1^2 + q_2^2 + \dots + q_N^2$  as in (3.21), or (ii) the one-dimensional case (3.12)–(3.17) with even functions

$$V(x) = V(-x) \quad \text{and} \quad h(x) = h(-x). \quad (4.2)$$

In the latter case, we need only to consider the region

$$x \equiv r \geq 0. \quad (4.3)$$

Thus, we need only to consider (i), since the  $N$ -dimensional radially symmetric solution (3.25) reduces to the one-dimensional case (3.15), with  $N = 1$  and  $r$  replaced by  $x$ . Furthermore, we assume  $h(r)$  to satisfy at all finite  $r > 0$ ,

$$h(r) > 0 \quad \text{and} \quad h'(r) < 0; \quad (4.4)$$

at infinity,

$$h(\infty) = 0. \quad (4.5)$$

Throughout the paper, ' denotes  $\frac{d}{dr}$ . An example of such  $h(r)$  is given in Appendix A for the quartic potential problem (1.3).

In accordance with (3.25), each  $n$ th iterative solution  $f_n(r)$  carries an independent additive constant. In the following, we differentiate two sets of sequences, labelled A and B, satisfying different boundary conditions:

$$f_n(\infty) = 1 \quad \text{for all } n \quad \text{in Case (A)} \quad (4.6)$$

or

$$f_n(0) = 1 \quad \text{for all } n \quad \text{in Case (B)}. \quad (4.7)$$

Thus, by using (3.25) or (3.32) we have in Case (A)

$$f_n(r) = 1 - 2 \int_r^\infty y^{-N+1} \phi^{-2}(y) dy \int_y^\infty z^{N-1} \phi^2(z) (h(z) - \mathcal{E}_n) f_{n-1}(z) dz, \tag{4.8A}$$

and in Case (B)

$$f_n(r) = 1 - 2 \int_0^r y^{-N+1} \phi^{-2}(y) dy \int_0^y z^{N-1} \phi^2(z) (h(z) - \mathcal{E}_n) f_{n-1}(z) dz. \tag{4.8B}$$

In both cases,  $\mathcal{E}_n$  is determined by the corresponding  $f_{n-1}(r)$  through (2.22); i.e.,

$$\mathcal{E}_n = [h f_{n-1}] / [f_{n-1}] \tag{4.9}$$

in which  $[F]$  of any function  $F(r)$  is defined to be

$$[F] = \int_0^\infty r^{N-1} \phi^2(r) F(r) dr. \tag{4.10}$$

It is convenient to introduce  $\chi(r)$  defined by

$$\chi(r) \equiv r^{(N-1)/2} \phi(r). \tag{4.11}$$

Thus, (4.10) becomes

$$[F] = \int_0^\infty \chi^2(r) F(r) dr. \tag{4.12}$$

Let  $\rho_n(r)$ ,  $\mathcal{K}(r)$  and  $\mathcal{D}_n(r)$  be related to  $\sigma_n(r)$ ,  $\kappa(r)$  and  $(D_n)_r$  of (3.2), (3.20) and (3.22) by

$$\rho_n(r) = r^{N-1} \sigma_n(r) = (h(r) - \mathcal{E}_n) \chi^2(r) f_{n-1}(r), \tag{4.13}$$

$$\mathcal{K}(r) = r^{N-1} \kappa(r) = \chi^2(r), \tag{4.14}$$

and

$$\mathcal{D}_n(r) = r^{N-1} (D_n)_r = -\frac{1}{2} \mathcal{K}(r) f'_n(r). \tag{4.15}$$

Correspondingly, in Case (A), (4.8A) can be written as

$$f_n(r) = 1 - 2 \int_r^\infty \chi^{-2}(y) dy \int_y^\infty \chi^2(z)(h(z) - \mathcal{E}_n) f_{n-1}(z) dz, \quad (4.16A)$$

and in Case (B), (4.8B) becomes

$$f_n(r) = 1 - 2 \int_0^r \chi^{-2}(y) dy \int_0^y \chi^2(z)(h(z) - \mathcal{E}_n) f_{n-1}(z) dz. \quad (4.16B)$$

Because of (3.23), we have

$$\mathcal{D}'_n(r) = \rho_n(r) \quad (4.17)$$

and therefore

$$\mathcal{D}_n(r) = - \int_r^\infty \rho_n(z) dz = - \int_r^\infty (h(z) - \mathcal{E}_n) \chi^2(z) f_{n-1}(z) dz. \quad (4.18)$$

From (3.7),

$$\int_0^\infty \rho_n(r) dr = 0 \quad (4.19)$$

which leads to

$$\mathcal{D}_n(r) = \int_0^r \rho_n(z) dz = \int_0^r (h(z) - \mathcal{E}_n) \chi^2(z) f_{n-1}(z) dz. \quad (4.20)$$

These two expressions of  $\mathcal{D}_n(r)$ , (4.18) and (4.20), are valid for both cases (A) and (B). Let  $r_n$  be defined by

$$h(r) - \mathcal{E}_n = 0 \quad \text{at } r = r_n. \quad (4.21)$$

Since  $h'(r) < 0$ , (4.21) has one and only one solution, with  $h(r) - \mathcal{E}_n$  negative for  $r > r_n$  and positive for  $r < r_n$ . Thus, if

$$f_{n-1}(r) > 0 \quad (4.22)$$

for all  $r > 0$ , we have from (4.18) and (4.20)

$$\mathcal{D}_n(r) > 0 \quad (4.23)$$

and therefore, on account of (4.15),

$$f'_n(r) < 0. \quad (4.24)$$

In Case (A), because of  $f_n(\infty) = 1$ , (4.24) leads to

$$f_n(0) > f_n(r) > f_n(\infty) = 1. \quad (4.25A)$$

Since for  $n=0$ ,  $f_0(r) = 1$ , (4.22)–(4.25A) are valid for  $n=1$ ; by induction these expressions also hold for all  $n$ ; in Case (A), their validity imposes no restriction on the magnitude of  $h(r)$ . In Case (B) we assume  $h(r)$  to be not too large, so that (4.16B) is consistent with

$$f_n(r) > 0 \quad \text{for all } r$$

and therefore

$$f_n(0) = 1 > f_n(r) > f_n(\infty) > 0. \quad (4.25B)$$

As we shall see, these two boundary conditions (A) and (B) produce sequences that have very different behavior. Yet, they also share a number of common properties.

*Hierarchy Theorem.* (A) With the boundary condition  $f_n(\infty) = 1$ , we have for all  $n$

$$\mathcal{E}_{n+1} > \mathcal{E}_n \quad (4.26)$$

and

$$\frac{d}{dr} \left( \frac{f_{n+1}(r)}{f_n(r)} \right) < 0 \quad \text{at any } r > 0. \quad (4.27)$$

Thus, the sequences  $\{\mathcal{E}_n\}$  and  $\{f_n(r)\}$  are all monotonic, with

$$\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3 < \dots \quad (4.28)$$

and

$$1 < f_1(r) < f_2(r) < f_3(r) < \dots \quad (4.29)$$



at all finite  $r$ .

(B) With the boundary condition  $f_n(0) = 1$ , we have for all odd  $n = 2m + 1$  an ascending sequence

$$\mathcal{E}_1 < \mathcal{E}_3 < \mathcal{E}_5 < \dots \tag{4.30}$$

but for all even  $n = 2m$ , a descending sequence

$$\mathcal{E}_2 > \mathcal{E}_4 > \mathcal{E}_6 > \dots, \tag{4.31}$$

furthermore, between any even  $n = 2m$  and any odd  $n = 2l + 1$

$$\mathcal{E}_{2m} > \mathcal{E}_{2l+1}. \tag{4.32}$$

Likewise, at any  $r$ , for any even  $n = 2m$

$$\frac{d}{dr} \left( \frac{f_{2m+1}(r)}{f_{2m}(r)} \right) < 0, \tag{4.33}$$

whereas for any odd  $n = 2l + 1$

$$\frac{d}{dr} \left( \frac{f_{2l+2}(r)}{f_{2l+1}(r)} \right) > 0. \tag{4.34}$$

The proof of the hierarchy theorem is given in Appendix B. The hierarchy theorem was discussed in our earlier papers for one-dimensional problems (18,19). The extension to the  $N$ -dimensional radially symmetric case is new. As we shall also discuss in Appendix B, the lowest eigenvalue  $E$  of the Hamiltonian  $T + V$  is the limit of the sequence  $\{E_n\}$  with

$$E_n = E_0 - \mathcal{E}_n. \tag{4.35}$$

Thus, the boundary condition  $f_n(\infty) = 1$  yields a sequence, in accordance with (4.28),

$$E_1 > E_2 > E_3 > \dots > E \tag{4.36}$$

with each member  $E_n$  an *upper* bound of  $E$ , similar to the usual variational method.

On the other hand, with the boundary condition  $f_n(0) = 1$ , while the sequence of its odd members  $n = 2l + 1$  yields a similar one, like (4.36), with

$$E_1 > E_3 > E_5 > \cdots > E, \quad (4.37)$$

its even members  $n = 2m$  satisfy

$$E_2 < E_4 < E_6 < \cdots < E. \quad (4.38)$$

It is unusual to have an iterative sequence of *lower* bounds of the eigenvalue  $E$ . Together, these sequences may be quite efficient to pinpoint the limiting  $E$ .

In Appendix C, we discuss the comparison between the iterative solution and perturbative series for some simple examples.

## 5. TRIBUTE

This paper is based on my joint work with Richard Friedberg. It was a pleasure for me to present the main body of the paper at the Number and Nature Symposium held on December 17–18, 2004 at the Rockefeller University, as a celebration for Mitchell J. Feigenbaum's 60th birthday. In the Chinese tradition, 60 is very special. It signifies the successful completion of one's first cycle, and the fresh beginning of a new second cycle.

Because China has no indigenous religion, there is no origin of reference in the Chinese calendar, nothing equivalent to BC or AD. All Chinese years are labelled cyclically, modulus sixty.

In Chinese calendar, each year is designated by two indices. The first index runs cyclically from 1 to 10, with each number represented by a different word shown in the first column of Chinese characters in Fig. 1. We may translate the first character at the top of that column as alpha (for 1) and the second character as beta (for 2), then gamma (for 3), ... until kappa (for 10); after kappa, we have alpha, beta, ... again. The second column of Chinese characters has 12 words, each for a different animal. In figure 1, the year 1944, when Mitchell was born is designated (Alpha-Monkey), the next year 1945 is (Beta-Chicken), ...; 10 years later, the first index for 1954 becomes again alpha, but the second index is horse; 2 years later for 1956, the first (number) index is gamma, but the second (animal) index becomes monkey again. It takes  $\frac{1}{2} \cdot 10 \cdot 12 = 60$  years

### Chinese Calender

(alpha)	甲	申	(monkey)	1944
(beta)	乙	酉	(chiken)	45
(gamma)	丙	戌	(dog)	46
.	.			
.	.			
(kappa)	癸	巳	(snake)	53
(alpha)	甲	午	(horse)	54
(beta)	乙	未	(sheep)	55
(gamma)	丙	申	(monkey)	56
	.	.		
	.	.		
	.	.		
(alpha)	甲	申	(monkey)	2004

Fig. 1. Chinese calender is cyclic, modulus sixty.

to complete the cycle. This year 2004 is like 1944, the Alpha-Monkey year and Mitchell is now in his new cycle, starting a new beginning.

The most beloved story in China is the book “Monkey” by Wu Cheng-En written in the 16th century. It is about an immortal Monkey-King of Chaos. The translation was by Arthur Waley (Fig. 2) in 1943, perhaps anticipating that 1944 was the beginning of Mitchell’s Alpha-Monkey cycle. To celebrate 2004, the beginning of Mitchell’s newest cycle, Fig. 3 is a drawing of mine, entitled “Monkey King the Thinker”. All of us are looking forward to this new cycle with our very best wishes.

# Monkey

## King of Chaos

Written by Wu Cheng-En

(16<sup>th</sup> Century)

Translated by Arthur Waley

(1943)

Fig. 2. One of the most beloved novels in China.

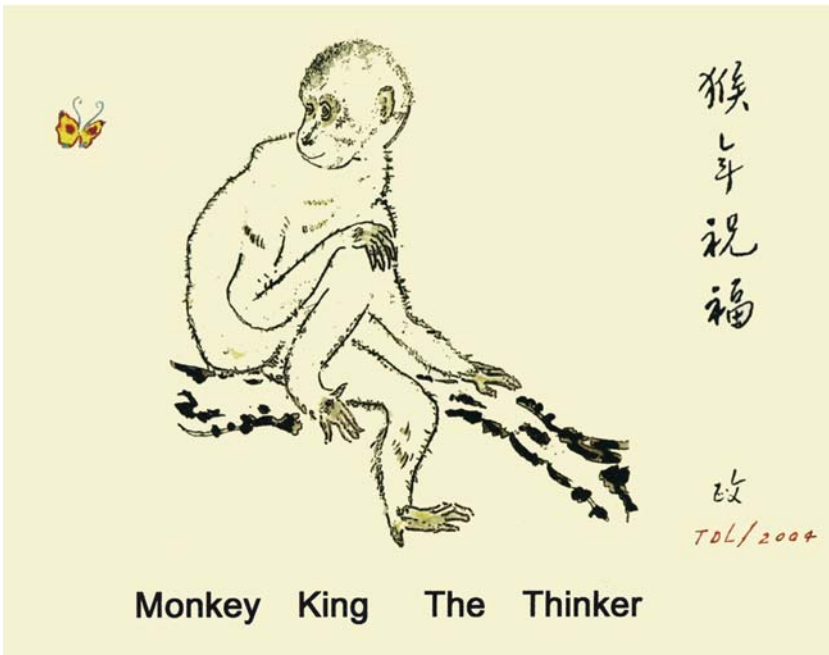


Fig. 3. “Monkey King the Thinker” by T. D. Lee (2004) (color online).

## APPENDIX A: CONSTRUCTION OF TRIAL FUNCTIONS

### A.1. A New Formulation of Perturbative Expansion

As mentioned in Section 1, in many problems of interest, perturbative expansion lead to asymptotic series. Nevertheless, the first few terms of

such an expansion could provide important insight to what a good trial function might be. For our purpose, a particularly convenient way is to follow the method developed in refs. 15 and 16. As we shall see, in this new method to each order of the perturbation, the wave function is always expressible in terms of a single line-integral in the  $N$ -dimensional coordinate space, which can be readily used for the construction of the trial wave function.

We begin with the Hamiltonian  $H$  in its standard form (2.1)–(2.3). Assume  $V(q)$  to be positive definite, and choose its minimum to be at  $q=0$ , with

$$V(q) \geq V(0) = 0. \tag{A.1}$$

Introduce a scale factor  $g^2$  by writing

$$V(q) = g^2 v(q) \tag{A.2}$$

and correspondingly

$$\psi(q) = e^{-gS(q)}. \tag{A.3}$$

Thus, the Schroedinger equation (2.4) becomes

$$\left( -\frac{1}{2}\nabla^2 + g^2 v(q) \right) e^{-gS(q)} = E e^{-gS(q)}, \tag{A.4}$$

where, as before,  $q$  denotes  $q_1, q_2, \dots, q_N$  and  $\nabla$  the corresponding gradient operator. Hence  $S(q)$  satisfies

$$-\frac{1}{2}g^2(\nabla S)^2 + \frac{1}{2}g\nabla^2 S + g^2 v = E. \tag{A.5}$$

Considering the case of large  $g$ , we expand

$$S(q) = S_0(q) + g^{-1}S_1(q) + g^{-2}S_2(q) + \dots \tag{A.6}$$

and

$$E = gE_0 + E_1 + g^{-1}E_2 + \dots \tag{A.7}$$

Substituting (A.6)–(A.7) into (A.5) and equating the coefficients of  $g^{-n}$  on both sides, we find

$$\begin{aligned}(\nabla S_0)^2 &= 2v, \\ \nabla S_0 \cdot \nabla S_1 &= \frac{1}{2} \nabla^2 S_0 - E_0, \\ \nabla S_0 \cdot \nabla S_2 &= \frac{1}{2} [\nabla^2 S_1 - (\nabla S_1)^2] - E_1, \\ \nabla S_0 \cdot \nabla S_3 &= \frac{1}{2} [\nabla^2 S_2 - 2 \nabla S_1 \cdot \nabla S_2] - E_2,\end{aligned}\tag{A.8}$$

etc. In this way, the second order partial differential equation (A.5) is reduced to a series of first order partial differential equations (A.8). The first of this set of equations can be written as

$$\frac{1}{2} [\nabla S_0(q)]^2 - v(q) = 0 +.\tag{A.9}$$

As noted in ref. 15, this is precisely the Hamilton–Jacobi equation of a single particle with unit mass moving in a potential “ $-v(q)$ ” in the  $N$ -dimensional  $q$ -space. Since  $q=0$  is the *maximum* of the classical potential energy function  $-v(q)$ , for any point  $q \neq 0$  there is always a classical trajectory with a total energy  $0+$ , which begins from  $q=0$  and ends at the other point  $q \neq 0$ , with  $S_0(q)$  given by the corresponding classical action integral. Furthermore,  $S_0(q)$  increases along the direction of the trajectory, which can be extended beyond the selected point  $q \neq 0$ , towards  $\infty$ . At infinity, it is easy to see that  $S_0(q) = \infty$ , and therefore the corresponding wave amplitude  $e^{-gS_0(q)}$  is zero. To solve the second equation in (A.8), we note that, in accordance with (A.1)–(A.2) at  $q=0$ ,  $\nabla S_0 \propto v^{\frac{1}{2}}(0) = 0$ . By requiring  $S_1(q)$  to be analytic at  $q=0$ , we determine

$$E_0 = \frac{1}{2} (\nabla^2 S_0)_{\text{at } q=0}.\tag{A.10}$$

It is convenient to consider the surface

$$S_0(q) = \text{constant};\tag{A.11}$$

its normal is along the corresponding classical trajectory passing through  $q$ . Characterize each classical trajectory by the  $S_0$ -value along the trajectory and a set of  $N-1$  angular variables

$$\alpha = (\alpha_1(q), \alpha_2(q), \dots, \alpha_{N-1}(q)),\tag{A.12}$$

so that each  $\alpha$  determines one classical trajectory with

$$\nabla\alpha_j \cdot \nabla S_0 = 0, \tag{A.13}$$

where

$$j = 1, 2, \dots, N - 1. \tag{A.14}$$

(As an example, we note that as  $q \rightarrow 0$ ,  $v(q) \rightarrow \frac{1}{2} \sum_i \omega_i^2 q_i^2$  and therefore  $S_0 \rightarrow \frac{1}{2} \sum_i \omega_i q_i^2$ . Consider the ellipsoidal surface  $S_0 = \text{constant}$ . For  $S_0$  sufficiently small, each classical trajectory is normal to this ellipsoidal surface. A convenient choice of  $\alpha$  could be simply any  $N - 1$  orthogonal parametric coordinates on the surface.) Each  $\alpha$  designates one classical trajectory, and vice versa. Every  $(S_0, \alpha)$  is mapped into a unique set  $(q_1, q_2, \dots, q_N)$  with  $S_0 \geq 0$  by construction. In what follows, we regard the points in the  $q$ -space as specified by the coordinates  $(S_0, \alpha)$ . Depending on the problem, the mapping  $(q_1, q_2, \dots, q_N) \rightarrow (S_0, \alpha)$  may or may not be one-to-one. We note that, for  $q$  near 0, different trajectories emanating from  $q = 0$  have to go along different directions, and therefore must associate with different  $\alpha$ . Later on, as  $S_0$  increases each different trajectory retains its initially different  $\alpha$ -designation; consequently, using  $(S_0, \alpha)$  as the primary coordinates, different trajectories never cross each other. The trouble-some complications of trajectory-crossing in  $q$ -space is automatically resolved by using  $(S_0, \alpha)$  as coordinates. Keeping  $\alpha$  fixed, the set of first order partial differential equations can be further reduced to a set of first order ordinary differential equations, which are readily solvable, as we shall see.

Write

$$S_1(q) = S_1(S_0, \alpha), \tag{A.15}$$

the second line of (A.8) becomes

$$(\nabla S_0)^2 \left( \frac{\partial S_1}{\partial S_0} \right)_\alpha = \frac{1}{2} \nabla^2 S_0 - E_0, \tag{A.16}$$

and leads to, besides (A.10), also

$$S_1(q) = S_1(S_0, \alpha) = \int_0^{S_0} \frac{dS_0}{(\nabla S_0)^2} \left[ \frac{1}{2} \nabla^2 S_0 - E_0 \right], \tag{A.17}$$

where the integration is taken along the classical trajectory of constant  $\alpha$ . Likewise, the third, fourth and other lines of (A.8) lead to

$$E_1 = \frac{1}{2}[\nabla^2 S_1 - (\nabla S_1)^2]_{\text{at } q=0}, \quad (\text{A.18})$$

$$S_2(q) = S_2(S_0, \alpha) = \int_0^{S_0} \frac{dS_0}{(\nabla S_0)^2} \left\{ \frac{1}{2}[\nabla^2 S_1 - (\nabla S_1)^2] - E_1 \right\}, \quad (\text{A.19})$$

$$E_2 = \frac{1}{2}[\nabla^2 S_2 - 2(\nabla S_1) \cdot (\nabla S_2)]_{\text{at } q=0}, \quad (\text{A.20})$$

$$S_3(q) = S_3(S_0, \alpha) = \int_0^{S_0} \frac{dS_0}{(\nabla S_0)^2} \left\{ \frac{1}{2}[\nabla^2 S_2 - 2(\nabla S_1) \cdot (\nabla S_2)] - E_2 \right\}, \quad (\text{A.21})$$

etc. These solutions give the convenient normalization convention at  $q=0$ ,

$$S(0) = 0$$

and

$$e^{-S(0)} = 1. \quad (\text{A.22})$$

### Remarks

(i) As an example, consider an  $N$ -dimensional harmonic oscillator with

$$V(q) = \frac{g^2}{2}(q_1^2 + q_2^2 + \cdots + q_N^2). \quad (\text{A.23})$$

From (A.2), one sees that the Hamilton–Jacobi equation (A.9) is for a particle moving in a potential given by

$$-v(q) = -\frac{1}{2}(q_1^2 + q_2^2 + \cdots + q_N^2). \quad (\text{A.24})$$

Thus, for any point  $q \neq 0$  the classical trajectory of interest is simply a straight line connecting the origin and the specific point, with the action

$$S_0(q) = \frac{1}{2}(q_1^2 + q_2^2 + \cdots + q_N^2). \quad (\text{A.25})$$



The corresponding energy is, in accordance with (A.10),

$$E_0 = \frac{N}{2}. \tag{A.26}$$

By using (A.8), one can readily show that  $E_1 = E_2 = \dots = 0$  and  $S_1 = S_2 = \dots = 0$ . The result is the well known exact answer with the groundstate wave function for the Schroedinger equation (A.4) given by

$$e^{-gS(q)} = \exp \left[ -\frac{g}{2} (q_1^2 + q_2^2 + \dots + q_N^2) \right] \tag{A.27}$$

and the corresponding energy

$$E = \frac{N}{2}g. \tag{A.28}$$

(ii) From this example, it is clear that the above expressions (A.6)–(A.8) are *not* the well-known WKB method. The new formalism uses  $-v(q)$  as the potential for the Hamilton–Jacobi equation, and its “classical” trajectory carries a  $0+$  energy; consequently, unlike the WKB method, there is no turning point along the classical trajectory, and the formalism is applicable to arbitrary dimensions.

### A.2. Trial Function for the Quantum Double-well Potential

To illustrate how to construct a trial function, consider the quartic potential (1.3) in one dimension with degenerate minima. Set  $a = 1$ , we have

$$V(x) = \frac{1}{2}g^2(x^2 - 1)^2. \tag{A.29}$$

The corresponding Schroedinger equation is

$$\left( -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}g^2(x^2 - 1)^2 \right) \psi(x) = E \psi(x), \tag{A.30}$$

where, as before,  $\psi(x) = e^{-gS(x)}$  is the groundstate wave function and  $E$  its energy. Using the expansions (A.6)–(A.7) and following the steps (A.8), (A.10) and (A.15)–(A.21), we find the well-known perturbative series

$$S_0(x) = \frac{1}{3}(x - 1)^2(x + 2), \quad S_1(x) = \ln \frac{x + 1}{2}, \quad S_2(x) = \frac{3}{16} - \frac{x + 2}{4(x + 1)^2}, \dots \tag{A.31}$$

and

$$E_0 = 1, \quad E_1 = -\frac{1}{4}, \quad E_2 = -\frac{9}{64}, \dots \tag{A.32}$$

Both expansions  $S = S_0 + g^{-1}S_1 + g^{-2}S_2 + \dots$  and  $E = gE_0 + E_1 + g^{-1}E_2 + \dots$  are divergent, furthermore, at  $x = -1$  and for  $n \geq 1$ , each  $S_n(x)$  is infinite. The reflection  $x \rightarrow -x$  gives a corresponding asymptotic expansion  $S_n(x) \rightarrow S_n(-x)$ , in which each  $S_n(-x)$  is regular at  $x = -1$ , but singular at  $x = +1$ .

As noted in Section 1, for  $g$  large, the first few terms of the perturbative series (with (A.31) for  $x$  positive and the corresponding expansion  $S_n(x) \rightarrow S_n(-x)$  for  $x$  negative) give a fairly good description of the true wave function  $\psi(x)$  whenever  $\psi(x)$  is large (i.e. for  $x$  near  $\pm 1$ ). However, for  $x$  near zero, when  $\psi(x)$  is exponentially small, the perturbative series becomes totally unreliable. This suggests the use of first few terms of the perturbative series for regions whenever  $\psi(x)$  is expected to be large. In regions where  $\psi(x)$  is exponentially small, simple interpolations by hand may already be adequate for a trial function, as we shall see. Since the quartic potential (A.29) is even in  $x$ , so is the groundstate wave function; likewise, we require the trial function  $\phi(x)$  also to satisfy  $\phi(x) = \phi(-x)$ . At  $x = 0$ , we require

$$\left(\frac{d\phi}{dx}\right)_{x=0} = 0. \tag{A.33}$$

To construct  $\phi(x)$ , we start with the first two functions  $S_0(x)$  and  $S_1(x)$  in (A.31). Introduce, for  $x \geq 0$ ,

$$\phi_+(x) \equiv e^{-gS_0(x) - S_1(x)} = \left(\frac{2}{1+x}\right) e^{-gS_0(x)} \tag{A.34}$$

and

$$\phi_-(x) \equiv e^{-gS_0(-x) - S_1(x)} = \left(\frac{2}{1+x}\right) e^{-\frac{4}{3}g + gS_0(x)}. \tag{A.35}$$

In order to satisfy (A.33), we define

$$\phi(x) = \phi(-x) \equiv \begin{cases} \phi_+(x) + \frac{g-1}{g+1}\phi_-(x) & \text{for } 0 \leq x < 1 \\ \left(1 + \frac{g-1}{g+1}e^{-\frac{4}{3}g}\right)\phi_+(x) & \text{for } x > 1 \end{cases} \tag{A.36}$$

Thus, by construction (A.33) is satisfied. Furthermore,  $\phi(x)$  is continuous everywhere, for  $x$  from  $-\infty$  to  $\infty$ , and so is its derivative.

By differentiating  $\phi_+(x)$  and  $\phi(x)$ , we see that they satisfy

$$(T + V + u)\phi_+ = g\phi_+ \tag{A.37}$$

and

$$(T + V + h)\phi = g\phi, \tag{A.38}$$

where

$$u(x) = \frac{1}{(1+x)^2} \tag{A.39}$$

and

$$h(x) = h(-x) \tag{A.40}$$

with, for  $x \geq 0$

$$h(x) = u(x) + \hat{g}(x) \tag{A.41}$$

where

$$\hat{g}(x) = \begin{cases} 2g \frac{(g-1)e^{2gS_0(x) - \frac{4}{3}g}}{(g+1) + (g-1)e^{2gS_0(x) - \frac{4}{3}g}} & \text{for } 0 \leq x < 1 \\ 0 & \text{for } x > 1. \end{cases} \tag{A.42}$$

Note that for  $g > 1$ ,  $\hat{g}(x)$  is positive, and has a discontinuity at  $x = 1$ . Furthermore, for  $x$  positive both  $u(x)$  and  $\hat{g}(x)$  are decreasing functions of  $x$ . Therefore,  $h(x)$  also satisfies (4.4) for  $x = r > 0$ .

**APPENDIX B: PROOF OF THE HIERARCHY THEOREM**

In this appendix, we give the proof of the Hierarchy Theorem stated in Section 4. The discussion follows very closely the one given for the one-dimensional case in ref. 19. We first establish several lemmas applicable to both boundary conditions (4.6) and (4.7): (A)  $f_n(\infty) = 1$  and (B)  $f_n(0) = 1$ .

**Lemma 1.** For any pair  $f_m(r)$  and  $f_l(r)$

$$(i) \text{ if at all } r, \quad \frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) < 0 \quad \text{then } \mathcal{E}_{m+1} > \mathcal{E}_{l+1}, \tag{B.1}$$

and

$$(ii) \text{ if at all } r, \quad \frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) > 0 \quad \text{then } \mathcal{E}_{m+1} < \mathcal{E}_{l+1}. \tag{B.2}$$

*Proof.* According to (4.9)

$$\mathcal{E}_{m+1}[f_m] = [h f_m]. \tag{B.3}$$

Also by definition (4.10),

$$\mathcal{E}_{l+1}[f_m] = [\mathcal{E}_{l+1} f_m]. \tag{B.4}$$

Their difference gives

$$(\mathcal{E}_{m+1} - \mathcal{E}_{l+1})[f_m] = [(h - \mathcal{E}_{l+1}) f_m]. \tag{B.5}$$

From (B.3),

$$0 = [(h - \mathcal{E}_{l+1}) f_l]. \tag{B.6}$$

Let  $r_{l+1}$  be defined by (4.21); i.e., at  $r = r_{l+1}$ ,

$$h(r_{l+1}) = \mathcal{E}_{l+1}. \tag{B.7}$$

Multiplying (B.5) by  $f_l(r_{l+1})$  and (B.6) by  $f_m(r_{l+1})$  and taking their difference, we have

$$f_l(r_{l+1})(\mathcal{E}_{m+1} - \mathcal{E}_{l+1})[f_m] = [(h - \mathcal{E}_{l+1}) (f_m(r) f_l(r_{l+1}) - f_l(r) f_m(r_{l+1}))], \tag{B.8}$$

in which the unsubscripted  $r$  acts as a dummy variable; thus  $[f_m(r)]$  means  $[f_m]$  and  $[f_m(r_{l+1})]$  means  $f_m(r_{l+1}) \cdot [1]$ , etc.

(i) If  $(f_m(r)/f_l(r))' < 0$ , then for  $r < r_{l+1}$

$$\frac{f_m(r)}{f_l(r)} > \frac{f_m(r_{l+1})}{f_l(r_{l+1})}. \tag{B.9}$$

In addition, since in accordance with (4.4) and (B.7),  $h'(r) < 0$  and  $h(r_{l+1}) = \mathcal{E}_{l+1}$ , we also have for  $r < r_{l+1}$

$$h(r) > \mathcal{E}_{l+1}. \tag{B.10}$$

Thus, the function inside the square bracket on the right hand side of (B.8) is positive for  $r < r_{l+1}$ . Also, the inequalities (B.9) and (B.10) both reverse their signs for  $r > r_{l+1}$ . Consequently, the right hand side of (B.8) is positive definite, and so is its left side. Therefore, on account of (4.25A)–(4.25B), (B.1) holds.

(ii) If  $(f_m(r)/f_l(r))' > 0$ , we see that for  $r < r_{l+1}$ , (B.9) reverses its sign but not (B.10). A similar reversal of sign happens for  $r > r_{l+1}$ . Thus, the right hand side of (B.8) is now negative definite and therefore  $\mathcal{E}_{m+1} < \mathcal{E}_{l+1}$ . Lemma 1 is proved.

Let

$$\eta = \eta(\xi) \tag{B.11}$$

be a single valued differentiable function of  $\xi$  in the range between  $a$  and  $b$  with

$$0 \leq a \leq \xi \leq b \tag{B.12}$$

and with

$$\eta(a) \geq 0. \tag{B.13}$$

**Lemma 2.** (i) The ratio  $\eta/\xi$  is a decreasing function of  $\xi$  for  $a < \xi < b$  if

$$\frac{d\eta}{d\xi} \leq \frac{\eta}{\xi} \quad \text{at } \xi = a \tag{B.14}$$

and

$$\frac{d^2\eta}{d\xi^2} < 0 \quad \text{for } a < \xi < b. \tag{B.15}$$

(ii) The ratio  $\eta/\xi$  is an increasing function of  $\xi$  for  $a < \xi < b$  if

$$\frac{d\eta}{d\xi} \geq \frac{\eta}{\xi} \quad \text{at } \xi = a \quad (\text{B.16})$$

and

$$\frac{d^2\eta}{d\xi^2} > 0 \quad \text{for } a < \xi < b. \quad (\text{B.17})$$

*Proof.* Define

$$L \equiv \xi \frac{d\eta}{d\xi} - \eta \quad (\text{B.18})$$

to be the Legendre transform  $L(\xi)$ . We have

$$\frac{dL}{d\xi} = \xi \frac{d^2\eta}{d\xi^2} \quad (\text{B.19})$$

and

$$\frac{d}{d\xi} \left( \frac{\eta}{\xi} \right) = \frac{L}{\xi^2}. \quad (\text{B.20})$$

Since (B.14) says that  $L(a) \leq 0$  and (B.15) says that  $\frac{dL}{d\xi} < 0$  for  $a < \xi < b$ , these two conditions imply  $L(\xi) < 0$  for  $a < \xi < b$ , which proves (i) in view of (B.20). The proof of (ii) is the same, but with inequalities reversed.

**Lemma 3.** For any pair  $f_m(r)$  and  $f_l(r)$

(i) if over all  $r$ ,

$$\frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) < 0 \quad \text{then at all } r, \quad \frac{d}{dr} \left( \frac{\mathcal{D}_{m+1}(r)}{\mathcal{D}_{l+1}(r)} \right) < 0, \quad (\text{B.21})$$

and (ii) if over all  $r$ ,

$$\frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) > 0 \quad \text{then at all } r, \quad \frac{d}{dr} \left( \frac{\mathcal{D}_{m+1}(r)}{\mathcal{D}_{l+1}(r)} \right) > 0. \quad (\text{B.22})$$

*Proof.* From (4.18) and (4.20), we have

$$\mathcal{D}'_{m+1}(r) = (h(r) - \mathcal{E}_{m+1}) \chi^2(r) f_m(r) \tag{B.23}$$

and

$$\mathcal{D}'_{l+1}(r) = (h(r) - \mathcal{E}_{l+1}) \chi^2(r) f_l(r). \tag{B.24}$$

Define

$$\xi = \mathcal{D}_{l+1}(r) \quad \text{and} \quad \eta = \mathcal{D}_{m+1}(r). \tag{B.25}$$

In any local region of  $r$  where  $\mathcal{D}'_{l+1}(r) \neq 0$ , we can regard  $\eta = \eta(\xi)$  through  $\eta(r) = \eta(\xi(r))$ . Hence, we have

$$\frac{d\eta}{d\xi} = \frac{\mathcal{D}'_{m+1}(r)}{\mathcal{D}'_{l+1}(r)} = R(r) \frac{f_m(r)}{f_l(r)}, \tag{B.26}$$

where

$$R(r) = \frac{h(r) - \mathcal{E}_{m+1}}{h(r) - \mathcal{E}_{l+1}}, \tag{B.27}$$

and

$$\begin{aligned} \frac{d}{d\xi} \left( \frac{d\eta}{d\xi} \right) &= \frac{1}{\mathcal{D}'_{l+1}} \left( \frac{\mathcal{D}'_{m+1}}{\mathcal{D}'_{l+1}} \right)' = \frac{1}{\mathcal{D}'_{l+1}} \left( R \frac{f_m}{f_l} \right)' \\ &= \frac{1}{\mathcal{D}'_{l+1}} \left( R' \frac{f_m}{f_l} + R \left( \frac{f_m}{f_l} \right)' \right) \end{aligned} \tag{B.28}$$

where

$$R'(r) = \frac{\mathcal{E}_{m+1} - \mathcal{E}_{l+1}}{(h(r) - \mathcal{E}_{l+1})^2} h'(r). \tag{B.29}$$

(i) If  $(f_m/f_l)' < 0$ , from Lemma 1, we have

$$\mathcal{E}_{m+1} > \mathcal{E}_{l+1}. \tag{B.30}$$

From  $h'(r) < 0$  and the definition of  $r_{m+1}$  and  $r_{l+1}$ , given by (B.7), we have

$$r_{m+1} < r_{l+1}, \tag{B.31}$$

$$h(r_{m+1}) = \mathcal{E}_{m+1} \quad \text{and} \quad h(r_{l+1}) = \mathcal{E}_{l+1}. \tag{B.32}$$

We note that from (4.18) and (4.20)  $\mathcal{D}_{m+1}(r)$  and  $\mathcal{D}_{l+1}(r)$  are both positive continuous functions of  $r$ , varying from at  $r=0$ ,

$$\mathcal{D}_{m+1}(0) = \mathcal{D}_{l+1}(0) = 0 \tag{B.33}$$

to at  $r = \infty$

$$\mathcal{D}_{m+1}(\infty) = \mathcal{D}_{l+1}(\infty) = 0 \tag{B.34}$$

with their maxima at  $r_{m+1}$  for  $\mathcal{D}_{m+1}(r)$  and  $r_{l+1}$  for  $\mathcal{D}_{l+1}(r)$ , since in accordance with (B.23)–(B.24) and (B.32),

$$\mathcal{D}'_{m+1}(r_{m+1}) = 0 \quad \text{and} \quad \mathcal{D}'_{l+1}(r_{l+1}) = 0. \tag{B.35}$$

From (B.29)–(B.30), we see that  $R'(r)$  is always  $< 0$ . Furthermore, from (B.27), we also find that the function  $R(r)$  has a discontinuity at  $r = r_{l+1}$ . At  $r = 0$ ,  $R(0)$  satisfies

$$0 < R(0) = \frac{h(0) - \mathcal{E}_{m+1}}{h(0) - \mathcal{E}_{l+1}} < 1. \tag{B.36}$$

As  $r$  increases from 0,  $R(r)$  decreases from  $R(0)$ , through

$$R(r_{m+1}) = 0, \tag{B.37}$$

to  $-\infty$  at  $r = r_{l+1}-$ ;  $R(r)$  then switches to  $+\infty$  at  $r = r_{l+1}+$ , and continues to decrease as  $r$  increases from  $r_{l+1}+$ . At  $r = \infty$ ,  $R(r)$  becomes

$$R(\infty) = \frac{\mathcal{E}_{m+1}}{\mathcal{E}_{l+1}} > 1. \tag{B.38}$$



**Table I. The Signs of  $\mathcal{D}'_{m+1}(r)$ ,  $\mathcal{D}'_{l+1}(r)$ ,  $h(r) - \mathcal{E}_{m+1}$ ,  $h(r) - \mathcal{E}_{l+1}$ ,  $R(r)$  and  $R'(r)$  in the Three Regions defined by (B.39), when  $\mathcal{E}_{m+1} > \mathcal{E}_{l+1}$**

Region	$\mathcal{D}'_{m+1}(r)$	$\mathcal{D}'_{l+1}(r)$	$h(r) - \mathcal{E}_{m+1}$	$h(r) - \mathcal{E}_{l+1}$	$R(r)$	$R'(r)$
I	$> 0$	$> 0$	$> 0$	$> 0$	$> 0$	$< 0$
II	$< 0$	$> 0$	$< 0$	$> 0$	$< 0$	$< 0$
III	$< 0$	$< 0$	$< 0$	$< 0$	$> 0$	$< 0$

It is convenient to divide the  $r$ -axis into three regions:

$$\begin{aligned}
 \text{(I)} \quad & 0 < r < r_{m+1}, \\
 \text{(II)} \quad & r_{m+1} < r < r_{l+1}, \\
 \text{(III)} \quad & r_{l+1} < r.
 \end{aligned}
 \tag{B.39}$$

The signs of  $\mathcal{D}'_{m+1}$ ,  $\mathcal{D}'_{l+1}$ ,  $R$  and  $R'$  in these regions are summarized in Table I. Assuming  $(f_m/f_l)' < 0$  we shall show the validity of (B.21),  $(\mathcal{D}_{m+1}/\mathcal{D}_{l+1})' < 0$ , in each of these three regions.

Since

$$\mathcal{E}_{l+1} < h(r) < \mathcal{E}_{m+1} \quad \text{in (II)},
 \tag{B.40}$$

$\mathcal{D}_{m+1}(r)$  is decreasing and  $\mathcal{D}_{l+1}(r)$  is increasing; it is clear that (B.21) holds in II.

In each of regions (I) and (III), we have  $R(r) > 0$  from (B.27) and  $R'(r) < 0$  from (B.29). Since  $(f_m/f_l)'$  is always negative by the assumption in (B.21), both terms inside the big parenthesis of (B.28) are negative; hence the same (B.28) states that  $d^2\eta/d\xi^2$  has the opposite sign from  $\mathcal{D}'_{l+1}$ . From the sign of  $\mathcal{D}'_{l+1}$  listed in Table I, we see that

$$\frac{d^2\eta}{d\xi^2} < 0 \quad \text{in (I)}
 \tag{B.41}$$

and

$$\frac{d^2\eta}{d\xi^2} > 0 \quad \text{in (III)}.
 \tag{B.42}$$

Within each region,  $\eta = \mathcal{D}_{m+1}(r)$  and  $\xi = \mathcal{D}_{l+1}(r)$  are both monotonic in  $r$ ; therefore,  $\eta$  is a single-valued function of  $\xi$  and we can apply Lemma 2.

In (I), at  $r=0$ , both  $\mathcal{D}_{m+1}(0)$  and  $\mathcal{D}_{l+1}(0)$  are 0 according to (4.20), but their ratio is given by

$$\frac{\mathcal{D}_{m+1}(0)}{\mathcal{D}_{l+1}(0)} = \frac{\mathcal{D}'_{m+1}(0)}{\mathcal{D}'_{l+1}(0)}. \tag{B.43}$$

Therefore,

$$\left(\frac{d\eta}{d\xi}\right)_{r=0} = \left(\frac{\eta}{\xi}\right)_{r=0}. \tag{B.44}$$

Furthermore, from (B.41),  $\frac{d^2\eta}{d\xi^2} < 0$  in (I), it follows from Lemma 2, case (i), the ratio  $\eta/\xi$  is a decreasing function of  $\xi$ . Since  $\xi' = \mathcal{D}'_{l+1}$  is  $> 0$  in (I) according to (B.24), we have

$$\frac{d}{dr} \left(\frac{\mathcal{D}_{m+1}}{\mathcal{D}_{l+1}}\right) < 0 \quad \text{in (I)}. \tag{B.45}$$

In (III), at  $r = \infty$ , both  $\mathcal{D}_{m+1}(\infty)$  and  $\mathcal{D}_{l+1}(\infty)$  are 0 according to (B.34). Their ratio is

$$\frac{\mathcal{D}_{m+1}(\infty)}{\mathcal{D}_{l+1}(\infty)} = \frac{\mathcal{D}'_{m+1}(\infty)}{\mathcal{D}'_{l+1}(\infty)}, \tag{B.46}$$

which gives at  $r = \infty$ ,

$$\left(\frac{d\eta}{d\xi}\right)_{r=\infty} = \left(\frac{\eta}{\xi}\right)_{r=\infty}. \tag{B.47}$$

As  $r$  decreases from  $r = \infty$  to  $r = r_{l+1}$ , from (B.42) we have  $\frac{d^2\eta}{d\xi^2} > 0$  in (III). It follows from Lemma 2, case (ii),  $\eta/\xi$  is an increasing function of  $\xi$ . Since  $\xi' = \mathcal{D}'_{l+1}$  is  $< 0$ , because  $r > r_{l+1}$ , we have

$$\frac{d}{dr} \left(\frac{\mathcal{D}_{m+1}}{\mathcal{D}_{l+1}}\right) < 0 \quad \text{in (III)}. \tag{B.48}$$

Thus, we prove case (i) of Lemma 3. Case (ii) of Lemma 3 follows from case (i) through the interchange of the subscripts  $m$  and  $l$ . Lemma 3 is then established.

**Lemma 4.** Take any pair  $f_m(r)$  and  $f_l(r)$

(A) For the boundary condition  $f_n(\infty) = 1$ , if at all  $r$ ,

$$\frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) < 0 \quad \text{then at all } r, \quad \frac{d}{dr} \left( \frac{f_{m+1}(r)}{f_{l+1}(r)} \right) < 0; \quad (\text{B.49A})$$

therefore, if at all  $r$ ,

$$\frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) > 0 \quad \text{then at all } r, \quad \frac{d}{dr} \left( \frac{f_{m+1}(r)}{f_{l+1}(r)} \right) > 0. \quad (\text{B.50A})$$

(B) For the boundary condition  $f_n(0) = 1$ , if at all  $r$ ,

$$\frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) < 0 \quad \text{then at all } r, \quad \frac{d}{dr} \left( \frac{f_{m+1}(r)}{f_{l+1}(r)} \right) > 0; \quad (\text{B.49B})$$

therefore, if at all  $r$ ,

$$\frac{d}{dr} \left( \frac{f_m(r)}{f_l(r)} \right) > 0 \quad \text{then at all } r, \quad \frac{d}{dr} \left( \frac{f_{m+1}(r)}{f_{l+1}(r)} \right) < 0. \quad (\text{B.50B})$$

*Proof.* Define

$$\hat{\xi} = f_{l+1}(r) \quad \text{and} \quad \hat{\eta} = f_{m+1}(r). \quad (\text{B.51})$$

From (4.15) we see that

$$\frac{d\hat{\eta}}{d\hat{\xi}} = \frac{f'_{m+1}(r)}{f'_{l+1}(r)} = \frac{\mathcal{D}_{m+1}(r)}{\mathcal{D}_{l+1}(r)} \quad (\text{B.52})$$

and

$$\frac{d}{d\hat{\xi}} \left( \frac{d\hat{\eta}}{d\hat{\xi}} \right) = \frac{1}{f'_{l+1}} \frac{d}{dr} \left( \frac{\mathcal{D}_{m+1}(r)}{\mathcal{D}_{l+1}(r)} \right). \quad (\text{B.53})$$

(A) In this case  $f_n(\infty) = 1$  for all  $n$ . Thus, at  $r = \infty$ ,  $\hat{\xi} = f_{l+1}(\infty) = 1$ ,  $\hat{\eta} = f_{m+1}(\infty) = 1$ , and their ratio

$$\left( \frac{\hat{\eta}}{\hat{\xi}} \right)_{r=\infty} = 1. \quad (\text{B.54})$$

At the same point  $r = \infty$ , in accordance with (4.18),  $\mathcal{D}_{l+1}(\infty) = \mathcal{D}_{m+1}(\infty) = 0$ , but their ratio is, on account of  $h(\infty) = 0$  and (B.1) of Lemma 1,

$$\frac{\mathcal{D}_{m+1}(\infty)}{\mathcal{D}_{l+1}(\infty)} = \frac{\mathcal{D}'_{m+1}(\infty)}{\mathcal{D}'_{l+1}(\infty)} = \frac{h(\infty) - \mathcal{E}_{m+1}}{h(\infty) - \mathcal{E}_{l+1}} = \frac{\mathcal{E}_{m+1}}{\mathcal{E}_{l+1}} > 1, \tag{B.55}$$

in which the last inequality follows from the same assumption, if  $(f_m/f_l)' < 0$ , shared by (B.1) of Lemma 1 and the present (B.49A) that we wish to prove. Thus, from (B.52), at  $r = \infty$

$$\left(\frac{d\hat{\eta}}{d\hat{\xi}}\right)_{r=\infty} = \frac{\mathcal{E}_{m+1}}{\mathcal{E}_{l+1}} > \left(\frac{\hat{\eta}}{\hat{\xi}}\right)_{r=\infty} = 1. \tag{B.56}$$

As  $r$  decreases from  $\infty$  to 0,  $\hat{\xi}$  increases from  $f_{l+1}(\infty) = 1$  to  $f_{l+1}(0) > 1$ , in accordance with (4.24) and (4.25A). On account of (B.21) of Lemma 3, we have  $(\mathcal{D}_{m+1}/\mathcal{D}_{l+1})' < 0$ , which when combined with (B.53) and  $f'_n(r) < 0$  leads to

$$\frac{d}{d\hat{\xi}} \left(\frac{d\hat{\eta}}{d\hat{\xi}}\right) > 0. \tag{B.57}$$

Thus, by using (B.16)–(B.17) of Lemma 2, we have  $\hat{\eta}/\hat{\xi}$  to be an increasing function of  $\hat{\xi}$ ; i.e.,

$$\frac{d}{d\hat{\xi}} \left(\frac{\hat{\eta}}{\hat{\xi}}\right) > 0. \tag{B.58}$$

Because

$$\frac{d}{dr} \left(\frac{\hat{\eta}}{\hat{\xi}}\right) = \hat{\xi}' \frac{d}{d\hat{\xi}} \left(\frac{\hat{\eta}}{\hat{\xi}}\right) = f'_{l+1} \frac{d}{d\hat{\xi}} \left(\frac{\hat{\eta}}{\hat{\xi}}\right) \tag{B.59}$$

and  $f'_{l+1} < 0$ , we find

$$\frac{d}{dr} \left(\frac{f_{m+1}}{f_{l+1}}\right) = \frac{d}{dr} \left(\frac{\hat{\eta}}{\hat{\xi}}\right) < 0, \tag{B.60}$$

which establishes (B.49A). Through the interchange of the subscripts  $m$  and  $l$ , we also obtain (B.50A).

Next, we turn to Case (B) with the boundary condition  $f_n(0) = 1$  for all  $n$ . Therefore at  $r = 0$ ,

$$\frac{f_{m+1}(0)}{f_{l+1}(0)} = 1. \tag{B.61}$$

Furthermore from (4.15) and (4.16B), we also have  $f'_{m+1}(0) = f'_{l+1}(0) = 0$  and  $\mathcal{D}_{m+1}(0) = \mathcal{D}_{l+1}(0) = 0$ , with their ratio given by

$$\begin{aligned} \left(\frac{df_{m+1}}{df_{l+1}}\right)_{r=0} &= \frac{f'_{m+1}(0)}{f'_{l+1}(0)} = \frac{\mathcal{D}_{m+1}(0)}{\mathcal{D}_{l+1}(0)} = \frac{\mathcal{D}'_{m+1}(0)}{\mathcal{D}'_{l+1}(0)} \\ &= \frac{h(0) - \mathcal{E}_{m+1}}{h(0) - \mathcal{E}_{l+1}}. \end{aligned} \tag{B.62}$$

From (B.1) of Lemma 1, we see that if  $(f_m/f_l)' < 0$ , then  $\mathcal{E}_{m+1} > \mathcal{E}_{l+1}$  and therefore

$$\left(\frac{df_{m+1}}{df_{l+1}}\right)_{r=0} < 1, \tag{B.63}$$

$$\left(\frac{\hat{\eta}}{\hat{\xi}}\right)_{r=0} = 1. \tag{B.64}$$

Thus,

$$\left(\frac{d\hat{\eta}}{d\hat{\xi}}\right)_{r=0} < \left(\frac{\hat{\eta}}{\hat{\xi}}\right)_{r=0}. \tag{B.65}$$

Analogously to (B.18), define

$$L(r) \equiv \hat{\xi} \frac{d\hat{\eta}}{d\hat{\xi}} - \hat{\eta} = f_{l+1}(r) \frac{f'_{m+1}(r)}{f'_{l+1}(r)} - f_{m+1}(r), \tag{B.66}$$

therefore

$$\begin{aligned} \frac{dL(r)}{dr} &= \hat{\xi}' \frac{dL}{d\hat{\xi}} = \hat{\xi}' \hat{\xi} \frac{d}{d\hat{\xi}} \frac{d\hat{\eta}}{d\hat{\xi}} \\ &= \hat{\xi} \frac{d}{dr} \left(\frac{d\hat{\eta}}{d\hat{\xi}}\right) = f_{l+1} \frac{d}{dr} \left(\frac{f'_{m+1}}{f'_{l+1}}\right) = f_{l+1} \frac{d}{dr} \left(\frac{\mathcal{D}_{m+1}}{\mathcal{D}_{l+1}}\right). \end{aligned} \tag{B.67}$$

From (B.21) of Lemma 3, we know that if  $(f_m/f_l)' < 0$  then  $(\mathcal{D}_{m+1}/\mathcal{D}_{l+1})' < 0$ , which leads to

$$\frac{dL(r)}{dr} < 0. \tag{B.68}$$

From (B.66), we have

$$L(r) = \hat{\xi} \left( \frac{d\hat{\eta}}{d\hat{\xi}} - \frac{\hat{\eta}}{\hat{\xi}} \right) = f_{l+1}(r) \left( \frac{d\hat{\eta}}{d\hat{\xi}} - \frac{\hat{\eta}}{\hat{\xi}} \right), \tag{B.69}$$

and therefore at  $r=0$ , because of (B.65),

$$L(0) < 0. \tag{B.70}$$

Combining (B.68) and (B.70), we derive

$$L(r) < 0 \quad \text{for } r \geq 0. \tag{B.71}$$

Multiplying (B.66) by  $f'_{l+1}(r)$ , we have

$$\begin{aligned} f'_{l+1}(r)L(r) &= f_{l+1}(r)f'_{m+1}(r) - f_{m+1}(r)f'_{l+1}(r) \\ &= f_{l+1}^2(r) \left( \frac{f_{m+1}(r)}{f_{l+1}(r)} \right)'. \end{aligned} \tag{B.72}$$

Because  $f'_{l+1}(r)$  and  $L(r)$  are both negative, it follows then

$$\left( \frac{f_{m+1}(r)}{f_{l+1}(r)} \right)' > 0,$$

which gives (B.49B) for Case (B), with the boundary condition  $f_n(0) = 1$ . Interchanging the subscripts  $m$  and  $l$ , (B.49B) becomes (B.50B), and Lemma 4 is established.

We now turn to the proof of the theorem stated in (4.26)–(4.34).

*Proof of the Hierarchy Theorem.* When  $n=0$ , we have

$$f_0(r) = 1. \tag{B.73}$$

From (4.22)–(4.24), we find for  $n = 1$

$$f_1'(r) < 0, \tag{B.74}$$

and therefore

$$(f_1/f_0)' < 0. \tag{B.75}$$

In Case (A), by using (B.49A) and by setting  $m = 1$  and  $l = 0$ , we derive  $(f_2/f_1)' < 0$ ; through induction, it follows then  $(f_{n+1}/f_n)' < 0$  for all  $n$ . From Lemma 1, we also find  $\mathcal{E}_{n+1} > \mathcal{E}_n$  for all  $n$ . Thus, (4.26)–(4.29) are established.

In Case (B), by using (B.75) and (B.49B), and setting  $m = 1$  and  $l = 0$ , we find  $(f_2/f_1)' > 0$ , which in turn leads to  $(f_3/f_2)' < 0, \dots$ , and (4.33)–(4.34). Inequalities (4.30)–(4.32) now follow from (B.1)–(B.2) of Lemma 1. The Hierarchy Theorem is proved.

Assuming that  $h(0)$  is finite, we have for any  $n$

$$0 < \mathcal{E}_n < h(0). \tag{B.76}$$

Therefore, each of the monotonic sequences

$$\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3 < \dots \quad \text{in (A)}$$

$$\mathcal{E}_1 < \mathcal{E}_3 < \mathcal{E}_5 < \dots \quad \text{in (B)}$$

and

$$\mathcal{E}_2 > \mathcal{E}_4 > \mathcal{E}_6 > \dots \quad \text{in (B)}$$

converges to a finite limit  $\mathcal{E}$ . By following the discussions in Section 5 of ref. 18, one can show that each of the corresponding monotonic sequences of  $f_n(r)$  also converges to a finite limit  $f(r)$ . The interchange of the limit  $n \rightarrow \infty$  and the integrations in (4.16A) completes the proof that in Case (A) the limits  $\mathcal{E}$  and  $f(r)$  satisfy

$$f(r) = 1 - 2 \int_r^\infty \chi^{-2}(y) dy \int_y^\infty \chi^2(z) (h(z) - \mathcal{E}) f(z) dz. \tag{B.77A}$$

As noted before, the convergence in Case (A) can hold for any large but finite and positive  $h(r)$ , provided that  $h'(r)$  is negative for  $r > 0$ . In Case

(B), a large  $h(r)$  may yield a negative  $f_n(r)$ , in violation of (4.25B). Therefore, the convergence does depend on the smallness of  $h(r)$ . One has to follow discussions similar to those given in Ref.17 to ensure that the limits  $\mathcal{E}$  and  $f(r)$  satisfy

$$f(r) = 1 - 2 \int_0^r \chi^{-2}(y) dy \int_0^y \chi^2(z) (h(z) - \mathcal{E}) f(z) dz. \quad (\text{B.77B})$$

## APPENDIX C: COMPARISON WITH PERTURBATIVE EXPANSION

### C.3. A Simple Model and its Iterative Solutions

Consider the one-dimensional problem in which  $V$ ,  $U$  and  $h$  of (2.1), (2.7) and (2.9) are given by

$$V(x) = V(-x) = \begin{cases} \infty & \text{for } |x| > L+l \\ 0 & \text{for } l < |x| < L+l, \\ -\frac{1}{2}g^2 & \text{for } |x| < l, \end{cases} \quad (\text{C.1})$$

$$U(x) = U(-x) = \begin{cases} \infty & \text{for } |x| > L+l, \\ 0 & \text{for } |x| < L+l \end{cases} \quad (\text{C.2})$$

and

$$h(x) = U(x) - V(x) = \begin{cases} 0 & \text{for } |x| > l, \\ \frac{1}{2}g^2 & \text{for } |x| < l. \end{cases} \quad (\text{C.3})$$

Let  $\phi(x)$  and  $\psi(x)$  be the respective groundstates of

$$H_0\phi = -\frac{1}{2} \frac{d^2\phi}{dx^2} + U\phi = E_0\phi \quad (\text{C.4})$$

and

$$H\psi = -\frac{1}{2} \frac{d^2\psi}{dx^2} + V\psi = E\psi. \quad (\text{C.5})$$



As a model, (C.5) is the Schroedinger equation that we wish to solve, and (C.4) is the equation that the trial function  $\phi$  satisfies. The iterative equation (2.19) becomes

$$\left(-\frac{1}{2} \frac{d^2}{dx^2} + U(x) - E_0\right) \psi_n(x) = (h(x) - \mathcal{E}_n) \psi_{n-1}(x). \tag{C.6}$$

with  $\psi_0 = \phi(x)$ . Since  $U$  and  $V$  are both even in  $x$ , we need only to consider the region

$$x \geq 0. \tag{C.7}$$

Set within  $x < L + l$

$$\phi(x) = \cos px \tag{C.8}$$

with

$$p(L + l) = \frac{\pi}{2} \quad \text{and} \quad E_0 = \frac{p^2}{2}. \tag{C.9}$$

Introduce, as in (2.25),  $f_n = \psi_n / \phi$ . We have in accordance with (3.1)–(3.7)

$$D_n(x) = -\frac{1}{2} \kappa(x) \frac{df_n}{dx}, \quad \kappa(x) = \phi^2(x), \tag{C.10}$$

$$\frac{dD_n}{dx} = \sigma_n(x) = (h(x) - \mathcal{E}_n) \phi^2(x) f_{n-1}(x), \tag{C.11}$$

$$\int_0^\infty \sigma_n(x) dx = 0 \tag{C.12}$$

and therefore

$$\mathcal{E}_n = \frac{\int_0^\infty h \phi^2 f_{n-1} dx}{\int_0^\infty \phi^2 f_{n-1} dx}. \tag{C.13}$$

One can verify that for  $n = 1$

$$\mathcal{E}_1 = \frac{g^2}{2(L+l)} \left( l + \frac{1}{2p} \sin 2pl \right), \quad (\text{C.14})$$

$$D_1(x) = \frac{g^2}{4(L+l)} \begin{cases} \left( l + \frac{\sin 2pl}{2p} \right) \left( L+l-x - \frac{\sin 2px}{2p} \right), & l < x < L+l, \\ \left( x + \frac{\sin 2px}{2p} \right) \left( L - \frac{\sin 2pl}{2p} \right), & 0 < x < l \end{cases} \quad (\text{C.15})$$

and

$$f_1(x) = \begin{cases} f_1(R) + \frac{\mathcal{E}_1}{p^2} [1 - p(L+l-x) \tan px], & l < x < L+l, \\ f_1(0) - \frac{1}{p} \left( \frac{g^2}{2} - \mathcal{E}_1 \right) x \tan px, & 0 < x < l. \end{cases} \quad (\text{C.16})$$

The constants  $f_1(R)$  and  $f_1(0)$  are related through the continuity of  $f_1(x)$  at  $x=l$ . In order to derive the general solution for  $f_n(x)$ , it is useful to consider a limited region in  $x$  (either  $|x| < l$  or  $|x| > l$ ) over which

$$\Delta_n \equiv 2(h(x) - \mathcal{E}_n) = \text{constant}. \quad (\text{C.17})$$

From (C.10)–(C.11), we have

$$-\frac{d}{dx} \left( \cos^2 px \frac{df_n}{dx} \right) = \Delta_n \cos^2 px f_{n-1}. \quad (\text{C.18})$$

Write

$$f_n = P_n(x) + (\tan px) Q_n(x). \quad (\text{C.19})$$

We find, from (C.18),

$$\begin{aligned} \frac{d^2}{dx^2} P_n + 2p \frac{d}{dx} Q_n &= -\Delta_n P_{n-1} \\ \frac{d^2}{dx^2} Q_n - 2p \frac{d}{dx} P_n &= -\Delta_n Q_{n-1}. \end{aligned} \quad (\text{C.20})$$

Thus,  $P_n$  and  $Q_n$  are both  $n$ th order polynomials in  $x$ . Define

$$P_n^\pm \equiv \frac{1}{2}(P_n \mp i Q_n) = (P_n^\mp)^*. \tag{C.21}$$

From (C.20),  $P_n^\pm$  satisfies

$$\left( \frac{d^2}{dx^2} \pm 2ip \frac{d}{dx} \right) P_n^\pm = -\Delta_n P_{n-1}^\pm. \tag{C.22}$$

It is useful to introduce a set of  $n$ th order polynomials  $R_n^\pm$ , independent of  $\Delta_n$ . We require

$$\left( \frac{d^2}{dx^2} \pm 2ip \frac{d}{dx} \right) R_n^\pm = -R_{n-1}^\pm \tag{C.23}$$

with the boundary conditions (i) for  $n=0$ ,

$$R_0^\pm(x) = 1 \quad \text{at all } x, \tag{C.24}$$

and (ii) for  $n > 0$ , at  $x=0$

$$R_n^\pm(0) = 0. \tag{C.25}$$

The solution for  $R_n^\pm(x)$  can be further simplified by introducing a set of  $n$ th order polynomials  $R_n(x|q)$  without the superscript  $+$  or  $-$ , but depending on a scaling parameter  $q$ , so that

$$R_n(x|q) = q^{2n} R_n\left(\frac{x}{q} \middle| 1\right), \tag{C.26}$$

where  $R_n(\frac{x}{q}|1)$  is an  $n$ th order polynomial of  $\frac{x}{q}$  with constant coefficients. The  $R_n(x|q)$  are related to  $R_n^\pm(x)$  defined by (C.23)–(C.25) through

$$\begin{aligned} R_n(x|q) &= R_n^+(x) & \text{when } q &= q^+ \equiv +\frac{i}{2p}, \\ R_n(x|q) &= R_n^-(x) & \text{when } q &= q^- \equiv -\frac{i}{2p}. \end{aligned} \tag{C.27}$$

Writing

$$u \equiv \frac{x}{q} \quad \text{and} \quad R_n\left(\frac{x}{q} \middle| 1\right) \equiv r_n(u), \tag{C.28}$$

we have

$$r_0(u) = 1, \quad r_1(u) = u, \quad r_2(u) = \frac{1}{2}u^2 + u,$$

$$r_3(u) = \frac{1}{6}u^3 + u^2 + 2u, \tag{C.29}$$

$$r_4(u) = \frac{1}{24}u^4 + \frac{1}{2}u^3 + \frac{5}{2}u^2 + 5u, \quad \text{etc.},$$

correspondingly

$$R_0(x|q) = 1, \quad R_1(x|q) = qx, \quad R_2(x|q) = \frac{1}{2}q^2x^2 + q^3x,$$

$$R_3(x|q) = \frac{1}{6}q^3x^3 + q^4x^2 + 2q^5x, \tag{C.30}$$

$$R_4(x|q) = \frac{1}{24}q^4x^4 + \frac{1}{2}q^5x^3 + \frac{5}{2}q^6x^2 + 5q^7x, \quad \text{etc.}$$

In terms of  $R_n^\pm(x)$ , the  $P_n^\pm(x)$  that satisfies (C.22) is given by

$$P_n^\pm(x) = \frac{1}{2} \Delta_1 \Delta_2 \cdots \Delta_n R_n^\pm(x) + c_1^\pm \Delta_2 \Delta_3 \cdots \Delta_n R_{n-1}^\pm(x) + c_2^\pm \Delta_3 \cdots \Delta_n R_{n-2}^\pm(x) + \cdots + c_{n-1}^\pm \Delta_n R_1^\pm(x) + c_n^\pm, \tag{C.31}$$

where  $c_1^\pm, c_2^\pm, \dots, c_n^\pm$  are integration constants, with  $c_m^\pm = (c_m^\mp)^*$  for all  $m$ . Thus for  $n = 1$ , since  $R_1(x|q) = qx$ ,

$$R_1^\pm(x) = R_1(x|q^\pm) = R_1\left(x \left| \pm \frac{i}{2p} \right. \right) = \pm \frac{ix}{2p}. \tag{C.32}$$

According to (C.31),

$$P_1^\pm(x) = \frac{1}{2} \Delta_1 R_1^\pm(x) + c_1^\pm = \pm \frac{ix}{4p} \Delta_1 + c_1^\pm \tag{C.33}$$

and from (C.21)

$$P_1 = P_1^+ + P_1^- = c_1^+ + c_1^-$$

and

$$Q_1 = i(P_1^+ - P_1^-) = -\frac{x}{2p} \Delta_1 + i(c_1^+ - c_1^-). \tag{C.34}$$

Since

$$\Delta_1 = 2(h(x) - \mathcal{E}_1) = \begin{cases} -2\mathcal{E}_1 & \text{for } l < x < L+l, \\ g^2 - 2\mathcal{E}_1 & \text{for } 0 < x < l, \end{cases} \tag{C.35}$$

we have, in agreement with (C.16),  $P_1$  is a constant in  $l < x < L+l$ , and a different constant in  $0 < x < l$ . Likewise,

$$Q_1 = \frac{\mathcal{E}_1 x}{p} + \text{constant} \quad \text{in } l < x < L+l \tag{C.36}$$

$$Q_1 = -\frac{1}{p} \left( \frac{g^2}{2} - \mathcal{E}_1 \right) x + \text{a different constant} \quad \text{in } 0 < x < l.$$

These integration constants are determined by the continuity equations between regions, leaving one final overall constant that is not determined. Likewise, we can derive the solution  $f_n(x)$  for any  $n$ .

If we impose the boundary condition at  $x = L+l$ ,

$$f_n(L+l) = 1, \tag{C.37}$$

then in accordance with the Hierarchy Theorem

$$\mathcal{E}_1 < \mathcal{E}_2 < \dots \tag{C.38}$$

with

$$\lim_{n \rightarrow \infty} \mathcal{E}_n = \mathcal{E} = E_0 - E \tag{C.39}$$

for any finite  $g^2$ .

**C.4. Analyticity of  $E(g^2)$**

The convergence of the perturbative series in  $g^2$  depends on, in the complex  $g^2$  plane, the location of the nearest singularity  $g_c^2$  of  $E(g^2)$  to the origin. While the simple model discussed above can be readily solved, it is more complicated to locate the singularities of  $E(g^2)$ . We first discuss the exact solution of (C.5). Again we need only consider the positive  $x$ -axis. Note that the well-depth  $-\frac{g^2}{2}$  has a critical value  $-\frac{g_0^2}{2}$ , for  $g^2 > g_0^2$ ,  $E < 0$ , and for  $g^2 < g_0^2$ ,  $E > 0$ . When  $g^2 = g_0^2$ ,  $E = 0$  and

$$\psi = \psi_c \propto \begin{cases} \frac{L+l-x}{L} & \text{for } l < x < L+l, \\ \cos q_0 x & \text{for } 0 < x < l \end{cases} \tag{C.40}$$

with

$$q_0 \tan q_0 l = \frac{1}{L}, \tag{C.41}$$

as required by the continuity of  $\psi'/\psi$  at  $x=l$ . When  $g^2 < g_0^2$ ,

$$\psi \propto \begin{cases} \sin[k(L+l-x)] & \text{for } l < x < L+l, \\ \cos qx & \text{for } 0 < x < l \end{cases} \tag{C.42}$$

with

$$q \tan ql = k \cot kL, \tag{C.43}$$

and

$$E = \frac{k^2}{2} = \frac{1}{2}(q^2 - g^2) > 0. \tag{C.44}$$

When  $g^2 > g_0^2$ ,

$$\psi \propto \begin{cases} \sinh[\kappa(L+l-x)] & \text{for } l < x < L+l, \\ \cos qx & \text{for } 0 < x < l \end{cases} \tag{C.45}$$

with

$$q \tan ql = \kappa \coth \kappa L \tag{C.46}$$

and

$$E = -\frac{\kappa^2}{2} = \frac{1}{2}(q^2 - g^2) < 0. \tag{C.47}$$

In the limit  $L \rightarrow \infty$ ,  $q_0 = 0$ , in accordance with (C.41), and therefore

$$g_0^2 = 0. \tag{C.48}$$

For any  $g^2$  however small,  $E$  is negative. Solution (C.45) becomes

$$\psi \propto \begin{cases} e^{-\kappa x} & \text{for } x > l, \\ \cos qx & \text{for } x < l \end{cases} \tag{C.49}$$

with

$$E = -\frac{\kappa^2}{2} = -\frac{1}{2}(g^2 - q^2) \tag{C.50}$$

and

$$\kappa = q \tan ql. \tag{C.51}$$

We examine the analyticity of  $E(g^2)$  for the case  $L = \infty$ , the same analysis can be extended to arbitrary  $L$ , but it is more complex. The singularities of  $E = E(g^2)$  can be determined by setting  $\frac{dE}{dg^2} = \infty$ ; i.e.,  $\frac{dg^2}{dE} = 0$ , which leads to, on account of  $E = -\frac{1}{2}\kappa^2$ ,

$$\frac{dg^2}{d\kappa^2} = 0. \tag{C.52}$$

Because  $g^2 = q^2 + \kappa^2$  according to (C.50), (C.52) is equivalent to  $\frac{dq^2}{d\kappa^2} + 1 = 0$ ; i.e.,

$$\frac{dq}{d\kappa} = -\frac{\kappa}{q}. \tag{C.53}$$

Differentiating (C.51), we find

$$\frac{d\kappa}{dq} = \tan ql + ql \sec^2 ql, \quad (\text{C.54})$$

which, when combined with (C.53), gives

$$-\frac{q}{\kappa} = \tan ql + ql \sec^2 ql. \quad (\text{C.55})$$

Since  $(q/\kappa) = \cot ql$  according to (C.51), (C.55) becomes

$$\cot ql + \tan ql + ql \sec^2 ql = 0;$$

i.e.,

$$\sec^2 ql(\cot ql + ql) = 0.$$

When  $\sec^2 ql = 0$ ,  $ql = \pm i\infty$  which is uninteresting for our purpose. Hence, for singularities at a finite  $g^2$ , we require

$$\cot ql + ql = 0, \quad (\text{C.56})$$

i.e.,

$$ql \tan ql = -1. \quad (\text{C.57})$$

Define

$$z = ql. \quad (\text{C.58})$$

Our problem is then reduced to the study of zeroes of

$$z \tan z + 1 = 0. \quad (\text{C.59})$$

For each zero at  $z$ , there is a singularity of  $E(g^2)$  in the complex  $g^2$  plane at  $g^2 = \kappa^2 + q^2 = q^2 \tan^2 ql + q^2$ ; i.e., at

$$g^2 l^2 = z^2 \tan^2 z + z^2 = 1 + z^2. \quad (\text{C.60})$$



(i) For  $z$  imaginary, we set  $z = \pm iy$ . (C.59) becomes  $y \tanh y = 1$ , which gives for the smallest  $|y| \cong 1.2$ ,  $z \cong \pm 1.2i$  and

$$g^2 l^2 \cong -0.44 . \tag{C.61}$$

As will be shown below, this gives  $g_c^2$ .

(ii) For  $z$  real, the nearest zeroes for (C.59) are  $z \cong \pm 2.8$  and correspondingly

$$g^2 l^2 \cong 8.8 . \tag{C.62}$$

(iii) We shall now establish that in the complex  $g^2$ -plane, the nearest singularity  $g_c^2$  of  $E(g^2)$  to the origin is given by (C.61); i.e.,

$$g_c^2 l^2 \cong -0.44 . \tag{C.63}$$

Consider the well known expansion

$$\tan z = 2z \sum_{n=0}^{\infty} \frac{1}{(n + \frac{1}{2})^2 \pi^2 - z^2} .$$

For  $z$  near  $\frac{\pi}{2}$ , we may write the righthand side as

$$\begin{aligned} & 2z \left[ \frac{1}{(\frac{\pi}{2})^2 - z^2} + \sum_{n=1}^{\infty} \frac{1}{(n + \frac{1}{2})^2 \pi^2 - z^2} \right] \\ &= 2z \left[ \frac{1}{(\frac{\pi}{2})^2 - z^2} + \sum_{n=1}^{\infty} \left( \frac{1}{(n + \frac{1}{2})^2 \pi^2} + \frac{z^2}{(n + \frac{1}{2})^4 \pi^4} + \dots \right) \right] \\ &= 2z \left[ \frac{1}{(\frac{\pi}{2})^2 - z^2} + \left( \frac{1}{2} - \frac{4}{\pi^2} \right) + z^2 \sum_{n=1}^{\infty} \frac{1}{(n + \frac{1}{2})^4 \pi^4} + \dots \right]. \tag{C.64} \end{aligned}$$

By using first the approximation

$$\tan z \cong 2z \left[ \frac{1}{(\frac{\pi}{2})^2 - z^2} + \left( \frac{1}{2} - \frac{4}{\pi^2} \right) \right] \tag{C.65}$$

and then the correction due to the successive remaining terms in (C.64), one can readily show that (C.61) gives the smallest singularity  $g_c^2$  in the  $g^2$ -plane. (Note that in this case, because  $L = \infty$ ,  $g_0 = 0$  in accordance with (C.48).) Thus, the perturbative series of  $E(g^2)$  is convergent only if  $g^2 l^2 < |g_c^2 l^2| \cong 0.44$ . On the other hand, the iterative series of Section C.1 is convergent for any finite  $g^2$ .

### C.3. A Comparative Study of Different Green's Functions

(i) Write the iterative equation (2.19) as

$$(H_0 - E_0)\psi_n(q) = S_n(q), \quad (\text{C.66})$$

where

$$S_n(q) = (h(q) - \mathcal{E}_n)\psi_{n-1}(q). \quad (\text{C.67})$$

In one dimension, setting  $q = x$  and using (2.25) and (3.15)–(3.16), the solution  $\psi_n(x)$  is given by

$$\psi_n(x) = \psi_n(\infty) + \int_{-\infty}^{\infty} (x|\mathcal{G}|z)S_n(z)dz, \quad (\text{C.68})$$

where the Green's function  $\mathcal{G}$  is

$$(x|\mathcal{G}|z) = -2\phi(x) \int_x^{\infty} \phi^{-2}(y)dy\theta(y-z)\phi(z) \quad (\text{C.69})$$

with

$$\theta(y-z) = \begin{cases} 1 & \text{for } z > y, \\ 0 & \text{for } z < y, \end{cases} \quad (\text{C.70})$$

and therefore

$$(x|\mathcal{G}|z) = 0 \quad \text{if } z < x. \quad (\text{C.71})$$

The function  $(x|\mathcal{G}|z)$  is one of the Sturm–Liouville family of Green's functions.<sup>(20)</sup> On the other hand, in deriving the usual perturbative series one deals often with similar equations of the form

$$(H_0 - \lambda)u(q) = v(q) \quad (\text{C.72})$$

where  $\lambda$  is a parameter. Let  $u_n$  be the  $n$ th member of the ortho-normal set of real eigenfunctions of  $H_0$  with eigenvalue  $e_n$ . We assume

$$\int u_n(q)u_m(q)d^Nq = \delta_{nm} = \begin{cases} 0, & n \neq m, \\ 1, & n = m. \end{cases} \tag{C.73}$$

Hence,

$$(H_0 - e_n)u_n(q) = 0 \tag{C.74}$$

which reduces to (2.8) when  $n=0$ ; i.e.,

$$e_0 = E_0 \quad \text{and} \quad u_0 = \phi. \tag{C.75}$$

For  $\lambda$  different from any of the eigenvalues  $e_n$ , the general solution of (C.72) is

$$u(q) = \int (q|G(\lambda)|\bar{q})v(\bar{q})d^N\bar{q}, \tag{C.76}$$

where

$$(q|G(\lambda)|\bar{q}) = \sum_n \frac{u_n(q)u_n(\bar{q})}{e_n - \lambda}. \tag{C.77}$$

To simplify our notations, we assume all  $u_n(q)$  to be real. When  $\lambda = E_0 = e_0$ , (C.72) becomes

$$(H_0 - e_0)u(q) = v(q), \tag{C.78}$$

same as (C.66). Since  $(H_0 - e_0)u_0 = 0$ , we have

$$\int u_0(q)v(q)d^Nq = 0. \tag{C.79}$$

The general solution of (C.78) is

$$u(q) = \int (q|\hat{G}(\lambda)|\bar{q})v(\bar{q})d^N\bar{q} + cu_0(q) \tag{C.80}$$

with  $c$  an arbitrary constant and

$$(q|\hat{G}(e_0)|\bar{q}) \equiv \sum_{n \neq 0} \frac{u_n(q)u_n(\bar{q})}{e_n - e_0}. \quad (\text{C.81})$$

In the subsection (iii) below, we shall analyze the difference between  $\mathcal{G}$  and  $G$ , or  $\hat{G}$ . Before that, we shall review the roles of  $G$  and  $\hat{G}$  in the usual perturbative formulas.

(ii) In order to solve the Schroedinger equation (2.4) perturbatively, we begin with (2.11); i.e.,

$$(H_0 - E_0)\psi(q) = (h - \mathcal{E})\psi(q). \quad (\text{C.82})$$

Following the standard Brillouin–Wigner procedure, we require

$$\int u_0(q)\psi(q)d^Nq = \int \phi(q)\psi(q)d^Nq = 1. \quad (\text{C.83})$$

Define

$$\hat{\psi}(q) = \psi(q) - u_0(q), \quad (\text{C.84})$$

which is orthogonal to  $u_0(q)$ , because of (C.83). Eq. (C.82) leads to

$$(H_0 - E_0)\hat{\psi}(q) = (h - \mathcal{E})(u_0(q) + \hat{\psi}(q)), \quad (\text{C.85})$$

on account of (2.10), this gives

$$(H_0 - E)\hat{\psi}(q) = (h - \mathcal{E})u_0(q) + h\hat{\psi}(q). \quad (\text{C.86})$$

Multiply (C.86) on the left by  $u_n$  and integrate. We have for  $n = 0$

$$\mathcal{E} = \int u_0 h(u_0 + \hat{\psi})d^Nq, \quad (\text{C.87})$$

the same as (2.16); for  $n \neq 0$

$$(e_n - E)(n|\hat{\psi}) = \int u_n h(u_0 + \hat{\psi})d^Nq, \quad (\text{C.88})$$

where

$$(n|\hat{\psi}) \equiv \int u_n \hat{\psi} d^N q. \tag{C.89}$$

Introduce the sequence

$$\hat{\psi}_1, \hat{\psi}_2, \hat{\psi}_3, \dots \tag{C.90}$$

with

$$(0|\hat{\psi}_l) = 0 \quad \text{for all } l \geq 1. \tag{C.91}$$

When  $l = 1$ , we require for all  $n \neq 0$

$$(e_n - E)(n|\hat{\psi}_1) = \int u_n h u_0 d^N q. \tag{C.92}$$

For  $l > 1$ ,

$$(e_n - E)(n|\hat{\psi}_l) = \int u_n h \hat{\psi}_{l-1} d^N q. \tag{C.93}$$

Therefore, the sum

$$\hat{\psi} = \sum_1^{\infty} \hat{\psi}_l \tag{C.94}$$

satisfies (C.86). In compact form,

$$\hat{\psi}(q) = \int (q|\hat{G}(E)|\bar{q}) \hat{S}(\bar{q}) d^N \bar{q}, \tag{C.95}$$

where

$$\hat{S}(q) = h \hat{\psi}(q) + (h - \mathcal{E})u_0(q). \tag{C.96}$$

The usual perturbative series can then be readily derived by first introducing a parameter  $\epsilon$ , defined by

$$h(q) = \epsilon \hat{h}(q). \tag{C.97}$$

The subsequent expansions of

$$E = E_0 + \epsilon E(1) + \epsilon^2 E(2) + \dots \quad (\text{C.98})$$

$$\hat{\psi}_l = \epsilon \hat{\psi}_l(1) + \epsilon^2 \hat{\psi}_l(2) + \dots \quad (\text{C.99})$$

and

$$\begin{aligned} \hat{G}(E) = & \hat{G}(E_0) + \epsilon E(1) \frac{\partial \hat{G}(E_0)}{\partial E_0} \\ & + \epsilon^2 \left[ E(2) \frac{\partial}{\partial E_0} + \frac{1}{2} (E(1))^2 \frac{\partial^2}{\partial E_0^2} \right] \hat{G}(E_0) + \dots \end{aligned} \quad (\text{C.100})$$

lead to the usual perturbative series.

(iii) According to (C.68)–(C.69), the Green's function  $\mathcal{G}$  satisfies

$$(H_0 - E_0)(x|\mathcal{G}|z) = \delta(x - z), \quad (\text{C.101})$$

whereas the function  $\hat{G}(E_0)$  given by (C.81) satisfies, in a one-dimensional problem,

$$(H_0 - E_0)(x|\hat{G}(E_0)|z) = \delta(x - z) - u_0(x)u_0(z) \quad (\text{C.102})$$

with  $u_0 = \phi$  in accordance with (C.75). Thus  $\mathcal{G}$  and  $\hat{G}$  are clearly different. As an explicit example, let

$$H_0 = -\frac{1}{2} \frac{d^2}{dx^2} + U(x) \quad (\text{C.103})$$

and

$$U(x) = \begin{cases} \infty & x > R, \\ 0 & 0 < x < R, \\ \infty & x < 0, \end{cases} \quad \text{for} \quad (\text{C.104})$$

similar to (C.2) and (C.4). The corresponding eigenfunction  $u_n(x)$  and eigenvalue  $e_n$  that satisfy (C.73)–(C.74) are

$$u_n = \sqrt{\frac{2}{R}} \sin k_n x \quad \text{and} \quad e_n = \frac{1}{2} k_n^2 \quad \text{with} \quad k_n = \frac{n+1}{R} \pi, \quad (\text{C.105})$$

and  $n = 0, 1, 2, \dots$ . For  $\lambda$  different from any of the eigenvalues  $e_n$ ,  $G(\lambda)$  of (C.77) in this one-dimensional problem is given by

$$(x|G(\lambda)|z) = \sum_{n=0}^{\infty} \frac{1}{e_n - \lambda} u_n(x)u_n(z), \tag{C.106}$$

where  $x$  and  $z$  can vary between 0 and  $R$ . Introduce

$$\chi_+ = \sin p(R - x), \quad \chi_- = \sin px, \tag{C.107}$$

$$\lambda = \frac{1}{2}p^2 \tag{C.108}$$

and

$$\omega = \left(\frac{d\chi_-}{dx}\right)\chi_+ - \left(\frac{d\chi_+}{dx}\right)\chi_- = p \sin pR. \tag{C.109}$$

The Green's function  $G(\lambda)$  can also be written as

$$(x|G(\lambda)|y) = \frac{2}{\omega} \begin{cases} \chi_-(x)\chi_+(y) & \text{for } x < y, \\ \chi_+(x)\chi_-(y) & \text{for } x > y. \end{cases} \tag{C.110}$$

One can readily verify that  $G(\lambda)$  satisfies

$$(x|G(\lambda)|y) = (y|G(\lambda)|x), \tag{C.111}$$

$$\left(-\frac{1}{2} \frac{d^2}{dx^2} + U(x)\right) (x|G(\lambda)|y) = \delta(x - y) \tag{C.112}$$

and the boundary conditions

$$(x|G(\lambda)|0) = (x|G(\lambda)|R) = 0. \tag{C.113}$$

As

$$\lambda \rightarrow e_0 = \frac{1}{2} \left(\frac{\pi}{R}\right)^2, \tag{C.114}$$

the Green's function  $\hat{G}(e_0)$  of (C.81) is given by

$$\begin{aligned} \hat{G}(e_0) &= \lim_{\lambda \rightarrow e_0} \left( G(\lambda) - \frac{1}{e_0 - \lambda} u_0(y)u_0(x) \right) \\ &= \sum_{n \neq 0} \frac{1}{e_n - e_0} u_n(y)u_n(x). \end{aligned} \tag{C.115}$$

Define

$$\phi(x) = \sin k_0 x \quad \text{and} \quad \hat{\phi}(x) = \cos k_0 x \tag{C.116}$$

with  $k_0 = \frac{\pi}{R}$ . We find

$$\begin{aligned} (x|\hat{G}|z) &= \frac{R}{\pi^2} \phi(x)\phi(z) - \frac{2}{\pi} \left( \phi(x)z\hat{\phi}(z) + \phi(z)x\hat{\phi}(x) \right) \\ &\quad + \frac{2R}{\pi} \cdot \begin{cases} \phi(x)\hat{\phi}(z) & \text{for } x < z, \\ \phi(z)\hat{\phi}(x) & \text{for } x > z. \end{cases} \end{aligned} \tag{C.117}$$

The function  $\mathcal{G}$  can also be expressed in terms of  $\phi$  and  $\hat{\phi}$ . We have

$$-\frac{R}{\pi} \hat{\phi}(x) = \phi(x) \int_{R/2}^x \frac{dy}{\phi^2(y)} \tag{C.118}$$

and

$$(x|\mathcal{G}|z) = \frac{2R}{\pi} \cdot \begin{cases} \phi(x)\hat{\phi}(z) - \phi(z)\hat{\phi}(x), & x < z, \\ 0, & x > z. \end{cases} \tag{C.119}$$

Thus,  $\mathcal{G}$  is related, but quite different from  $\hat{G}$  and  $G$ .

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