New Ways to Solve the Schroedinger Equation∗

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Abstract

We discuss a new approach to solve the low lying states of the Schroedinger equation. For a fairly large class of problems, this new approach leads to convergent iterative solutions, in contrast to perturbative series expansions. These convergent solutions include the long standing difficult problem of a quartic potential with either symmetric or asymmetric minima.

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1. Introduction

Quantum physics is largely governed by the Schrödinger equation. Yet, exact solutions of the equation are relatively few. Besides lattice and other numerical calculations, we rely mostly on perturbative expansions. Such expansion quite often leads to a divergent series with zero radius of convergence, as in quantum electrodynamics, quantum chromodynamics and problems involving tunnelling and instantons. In a series of previous papers [1-4] we have presented a new approach to solve the low lying states of the Schrödinger equation. In the special case of one dimensional problems, this new approach leads to explicit convergent iterative solutions, in contrast to perturbative series expansions. These convergent solutions include the long standing difficult problem [5-14] of a quartic potential with symmetric minima.

In this paper, we discuss some additional results bearing on the new method. In the one-dimensional case, we show that by changing the boundary condition to be applied at each iteration, we can obtain a convergent alternating sequence for the groundstate energy and wave function instead of the monotonic sequence found before [4]. This result will be spelled out later in this section and proved in Section 3. We also find that the asymmetric quartic double-well potential can be treated by an extension of the procedure used previously for the symmetric case. This extension is treated in Section 4.

In addition, we have begun the exploration of higher dimensional problems along the same line. Although the same kind of iterative procedure can be set up, the linear inhomogeneous equation to be solved at each step cannot now be reduced to simple quadratures, as was done for one dimension. However, it is of interest that this equation is identical in form to an electrostatic analog problem with a given position dependent dielectric constant media; at each nth iteration, there is an external electrostatic charge distribution determined by the (n − 1)th iterated solution, as we shall discuss in this section.

Consider the Schrödinger equation

\[ H\psi = E\psi \]  

(1.1)

where \( H \) is the Hamiltonian operator, \( \psi \) the wave function and \( E \) its energy. For different physics problems, \( H \) assumes different forms. For example, for a system of \( n \) non-relativistic particles in three dimensions, \( H \) may be written as

\[ H = \sum_{i,j} C_{ij} p_i p_j + V(x) \]  

(1.2)

where \( x \) stands for \( x_1, x_2, \cdots, x_{3n} \) the coordinate components of these \( n \) particles, \( V(x) \) is the potential function, \( C_{ij} \) are constants and \( p_1, p_2, \cdots, p_{3n} \) are the momentum operators satisfying the commutation relation

\[ [p_i, x_j] = -i\delta_{ij}. \]  

(1.3)

(Throughout the paper, we set Planck’s constant \( \hbar = 1 \).) For a relativistic field theory, the Hamiltonian usually takes on a different form. Let \( \Phi(r) \) be a scalar boson field at a three-dimensional position vector \( r \), and \( \Pi(r) \) be the corresponding conjugate momentum operator.
In this case we may write

\[ H = \int d^3r [\Pi^2(r) + V(\Phi(r))] \]  \hspace{1cm} (1.4)

with \( \Pi(r) \) and \( \Phi(r') \) satisfying the commutation relation

\[ [\Pi(r), \Phi(r')] = -i\delta^3(r - r'). \]  \hspace{1cm} (1.5)

In both cases, the dependence of \( H \) on the momentum operators \( p_i \) and \( \Pi(r) \) are quadratic. Consequently, they can be brought into an identical standard form. In the above case of a system of non-relativistic particles, through a linear transformation

\[ \{x_i\} \rightarrow \{q_i\}, \]  \hspace{1cm} (1.6)

the Hamiltonian (1.2) can be written in the standard form

\[ H = -\frac{1}{2}\nabla^2 + V(q_1, q_2, \cdots, q_N) \]  \hspace{1cm} (1.7)

with

\[ \nabla^2 = \sum_{i=1}^{N} \frac{\partial^2}{\partial q_i^2}. \]  \hspace{1cm} (1.8)

Likewise for the relativistic boson field Hamiltonian (1.4), we can use the Fourier-components of \( \Phi(r) \) and \( \Pi(r) \) as the set \( \{x_i\} \) and \( \{p_i\} \). Through a similar transformation (1.6), the field Hamiltonian (1.4) can also be brought into the standard form (1.7) and (1.8), but with the number of variables \( N = \infty \). All our subsequent discussions will start from the Schroedinger equation in this standard form (1.7) - (1.8). Furthermore, in this paper, we shall limit our discussions only to the groundstate.

In order to solve

\[ (-\frac{1}{2}\nabla^2 + V(q))\psi(q) = E\psi(q) \]  \hspace{1cm} (1.9)

where \( q \) stands for the set \( \{q_i\} \), we proceed as follows:

1. Construct a good trial function \( \phi(q) \). A rather efficient way to find such trial functions is given in the next section.

2. By differentiating \( \phi \), we define

\[ U(q) - E_0 \equiv \phi(q)^{-1}(\frac{1}{2}\nabla^2\phi(q)), \]  \hspace{1cm} (1.10)

in which the constant \( E_0 \) may be determined by, e.g., setting the minimum value of \( U(q) \) to be zero. Thus, \( \phi(q) \) satisfies a different Schroedinger equation

\[ (-\frac{1}{2}\nabla^2 + U(q)\phi(q) = E_0\phi(q). \]  \hspace{1cm} (1.11)
Define \( w(q) \) and \( \mathcal{E} \) by
\[
U(q) = V(q) + w(q)
\] (1.12)
and
\[
E_0 = E + \mathcal{E}.
\] (1.13)

The original Schroedinger equation (1.9) can then be written as
\[
(-\frac{1}{2} \nabla^2 + U(q) - E_0)\psi(q) = (w(q) - \mathcal{E})\psi(q).
\] (1.14)

Multiplying this equation on the left by \( \phi(q) \) and (1.11) by \( \psi(q) \), we find their difference to be
\[
-\frac{1}{2} \nabla \cdot (\phi \nabla \psi - \psi \nabla \phi) = (w - \mathcal{E})\psi\phi.
\] (1.15)

The integration of its lefthand side over all space is zero, which yields
\[
\mathcal{E} = \frac{\int w\psi\phi \, d^N q}{\int \psi\phi \, d^N q}.
\] (1.16)

3. The above equation (1.14) will be solved iteratively by considering the sequences
\[
\psi_1, \psi_2, \cdots, \psi_n, \cdots \quad \text{and} \quad \mathcal{E}_1, \mathcal{E}_2, \cdots, \mathcal{E}_n, \cdots
\] (1.17)
that satisfy
\[
(-\frac{1}{2} \nabla^2 + U(q) - E_0)\psi_n(q) = (w(q) - \mathcal{E}_n)\psi_{n-1}(q)
\] (1.18)
with
\[
\psi_0(q) = \phi(q).
\] (1.19)

As in (1.15) and (1.16), we multiply (1.11) by \( \psi_n \) and (1.18) by \( \phi \); their difference gives
\[
-\frac{1}{2} \nabla \cdot (\phi \nabla \psi_n - \psi_n \nabla \phi) = (w - \mathcal{E}_n)\psi_{n-1}\phi
\] (1.20)
and therefore
\[
\mathcal{E}_n = \frac{\int w\psi_{n-1}\phi \, d^N q}{\int \psi_{n-1}\phi \, d^N q}.
\] (1.21)

As we shall show, for many interesting problems
\[
\lim_{n \to \infty} \mathcal{E}_n = \mathcal{E} \quad \text{and} \quad \lim_{n \to \infty} \psi_n = \psi,
\] (1.22)
in contrast to the perturbative series expansion using $w(q)$ as the perturbation. The key difference lies in the above expression (1.21) of $E_n$, which is a ratio, with both its numerator and denominator depending on the $(n-1)^{th}$ iterative solution $\psi_{n-1}$.

4. There exists a simple electrostatic analog problem for the iterative equation (1.18). Assuming that $\psi_{n-1}(q)$ has already been solved, we can determine $E_n$ through (1.21). The righthand side of (1.20), defined by

$$\sigma_n(q) \equiv (w(q) - E_n)\psi_{n-1}(q)\phi(q),$$

is then a known function. Introduce

$$f_n(q) \equiv \psi_n(q)/\phi(q).$$

In terms of $f_n(q)$, the $n^{th}$ order iterative equation (1.20) becomes

$$-\frac{1}{2} \nabla \cdot (\phi^2 \nabla f_n) = \sigma_n.$$  \hspace{1cm} (1.25)

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

$$\kappa(q) \equiv \phi^2(q).$$  \hspace{1cm} (1.26)

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

$$D_n \equiv -\frac{1}{2} \kappa \nabla f_n$$  \hspace{1cm} (1.27)

the corresponding displacement vector field. Thus (1.25) becomes

$$\nabla \cdot D_n = \sigma_n,$$  \hspace{1cm} (1.28)

the Maxwell equation for this electrostatic analog problem.

At infinity, $\phi(\infty) = 0$. In accordance with (1.26) - (1.27), we also have $D_n(\infty) = 0$. Hence the integration of (1.28) leads to the total external electrostatic charge to be also zero; i.e.,

$$\int \sigma_n(q) \, d^Nq = 0$$  \hspace{1cm} (1.29)

which is the same result given by (1.21) for the determination of $E_n$. Because the dielectric constant $\kappa(q)$ in this analog problem is zero at $q = \infty$, the dielectric media becomes a perfect dielectric at $\infty$. Thus, the equation of zero total charge, given by (1.29), may serve as a much simplified model of charge confinement, analogous to color confinement in quantum chromodynamics.

We note that (1.25) can also be derived from a minimal principle by defining

$$I(f_n(q)) \equiv \int \left\{ \frac{1}{4} \kappa(\nabla f_n)^2 + \sigma_n f_n \right\} d^Nq.$$  \hspace{1cm} (1.30)
Because of (1.29), the functional \( I(f_n(q)) \) is invariant under
\[
f_n(q) \rightarrow f_n(q) + \text{constant.} \tag{1.31}
\]

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 (1.25), with the same \( \kappa = \phi^2 \) and the same \( \sigma_n \); their difference would then satisfy (1.25) 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 we shall show, this arbitrariness allows us the freedom to derive different types of convergent series.

To illustrate this freedom, let us consider a one-dimensional problem in which we may replace the variables \( \{q_i\} \) by a single \( x \). Furthermore, for this discussion, let us assume the potential \( V(x) \) to be an even function, with
\[
V(x) = V(-x) \tag{1.32}
\]
(a condition that will be relaxed in our later analysis). The evenness of \( V(x) \) requires \( \psi(x) = \psi(-x) \) and therefore also \( \phi(x) = \phi(-x) \). Thus, we need only to consider the half-space
\[
x \geq 0. \tag{1.33}
\]

Equations (1.24), (1.27) and (1.28) can be written now as
\[
f_n(x) = \frac{\psi_n(x)}{\phi(x)}, \tag{1.34}
\]
\[
D_n = -\frac{1}{2}\kappa(x)f_n'(x) \tag{1.35}
\]
and
\[
D_n'(x) = \sigma_n(x) \tag{1.36}
\]
where
\[
\kappa(x) = \phi^2(x) \tag{1.37}
\]
and
\[
\sigma_n(x) = (w(x) - E_n)\phi(x)\psi_{n-1}(x) \tag{1.38}
\]
same as before. Throughout the paper, \( \cdot \) denote \( \frac{d}{dx} \).
From (1.36) and $D_n(\infty) = 0$, we have

$$D_n(x) = -\int_x^{\infty} \sigma_n(z)\,dz$$  \hspace{1cm} (1.39)

and, since $\sigma_n(x)$ is even in $x$, we have from (1.29),

$$\int_0^{\infty} \sigma_n(z)\,dz = 0.$$  \hspace{1cm} (1.40)

It follows then from (1.34) and (1.38)-(1.40),

$$D_n(x) = -\int_0^{\infty} \sigma_n(z)\,dz$$  \hspace{1cm} (1.41)

which lead to, through (1.35),

$$f_n(x) = f_n(\infty) - 2\int_0^{\infty} \phi^{-2}(y) \int_0^{\infty} \phi^2(z)(w(z) - E_n)\,f_{n-1}(z)\,dz$$  \hspace{1cm} (1.42)

and

$$f_n(x) = f_n(0) - 2\int_0^{x} \phi^{-2}(y) \int_0^{\infty} \phi^2(z)(w(z) - E_n)\,f_{n-1}(z)\,dz.$$  \hspace{1cm} (1.43)

Consider first the case that $w(x)$ in (1.38) is positive and satisfies

$$w'(x) < 0 \quad \text{for} \quad x > 0.$$  \hspace{1cm} (1.44)

The hierarchy theorem that will be proved in Section 3 states that if $w(x)$ satisfies (1.44) then the iterative solution of (1.42) with the boundary condition

$$f_n(\infty) = 1 \quad \text{for all} \quad n$$  \hspace{1cm} (1.45)

gives a convergent monotonic sequence $E_1, E_2, E_3, \ldots$, where for all $n$,

$$E_n > E_{n-1},$$  \hspace{1cm} (1.46)

and

$$E_n \rightarrow E \quad \text{as} \quad n \rightarrow \infty;$$  \hspace{1cm} (1.47)

likewise, the sequence $f_0(x) = 1, f_1(x), f_2(x), \ldots$ is also monotonic and convergent at any $x \geq 0$ with

$$f_n(x) > f_{n-1}(x).$$  \hspace{1cm} (1.48)
and
\[ f_n(x) \to f(x) \quad \text{as} \quad n \to \infty. \]  
(1.49)

Furthermore, the convergence of (1.47) and (1.49) can hold for arbitrarily large but finite \( w(x) \). A result that is surprising, but pleasant.

On the other hand, if instead of (1.45), we impose a different boundary condition, one given by
\[ f_n(0) = 1 \quad \text{for all} \quad n, \]  
(1.50)
then instead of (1.47), we have for all odd \( n = 2m + 1 \) an ascending sequence
\[ \mathcal{E}_1 < \mathcal{E}_3 < \mathcal{E}_5 < \cdots; \]  
(1.51)
however, for the even \( n = 2m \) series, we have a descending sequence
\[ \mathcal{E}_2 > \mathcal{E}_4 > \mathcal{E}_6 > \cdots; \]  
(1.52)
furthermore, between any even \( n = 2m \) and any odd \( n = 2l + 1 \), we have
\[ \mathcal{E}_{2m} > \mathcal{E}_{2l+1}. \]  
(1.53)

Since according to (1.13), \( \mathcal{E}_n \) is the \( n^{th} \) order iteration towards
\[ \mathcal{E} = E_0 - E, \]  
(1.54)
each odd member \( \mathcal{E}_{2l+1} \) in (1.51) gives an upper bound of \( E \), whereas each even member \( \mathcal{E}_{2m} \) in (1.52) leads to a lower bound of \( E \). Both sequences approach the correct \( \mathcal{E} \) as \( n \to \infty \), one from above and the other from below. For the boundary condition (1.50), our proof of convergence requires a condition on the magnitude of \( w(x) \). Still this is quite a remarkable result.

In Section 2, we discuss the details of how to construct a good trial function \( \phi(q) \) for the \( N \)-dimensional problem. Section 3 gives the proof of the hierarchy theorem for the one-dimensional problem in which \( V(x) = V(-x) \) is an even function of \( x \) and the potential-difference function \( w(x) \) is assumed to satisfy (1.44); i.e., \( w'(x) < 0 \) for \( x > 0 \). The extension to the asymmetric case \( V(x) \neq V(-x) \) is discussed in Section 4. The hierarchy theorem is also applicable to Mathieu’s equation, which has infinite number of maxima and minima. In the Appendix, we give a soluble example in one dimension.

In dimensions greater than 1, at each iteration Eq.(1.21) gives a fine tuning of the energy, just like the one-dimensional problem. Hence, there are good reasons to expect our approach to yield convergent solutions in any higher dimension. In Section 5, we formulate an explicit conjecture to this effect. We describe an attempt to prove this conjecture by generalizing the steps used to prove the hierarchy theorem in one dimension. The attempt fails at present because the proof of one of the lemmas does not appear to generalize in higher dimension.

The present paper represents the synthesis and generalization of results, some of which have appeared in our earlier publications[1-4]. The function \( D_n \) introduced in this paper is identical to the function \( h_n \) used in Ref.[4].
2. Construction of Trial Functions

2.1 A New Formulation of Perturbative Expansion

In many problems of interest, perturbative expansion leads to asymptotic series, which is not the aim of this paper. 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. [1] and [2]. 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 (1.7). Assume $V(q)$ to be positive definite, and choose its minimum to be at $q = 0$, with

$$V(q) \geq V(0) = 0. \quad (2.1)$$

Introduce a scale factor $g^2$ by writing

$$V(q) = g^2 v(q) \quad (2.2)$$

and correspondingly

$$\psi(q) = e^{-gS(q)}. \quad (2.3)$$

Thus, the Schrödinger equation (1.9) becomes

$$(-\frac{1}{2} \nabla^2 + g^2 v(q))e^{-gS(q)} = E e^{-gS(q)} \quad (2.4)$$

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

$$-\frac{1}{2} g^2 (\nabla S)^2 + \frac{1}{2} g \nabla^2 S + g^2 v = E. \quad (2.5)$$

Considering the case of large $g$, we expand

$$S(q) = S_0(q) + g^{-1} S_1(q) + g^{-2} S_2(q) + \cdots \quad (2.6)$$

and

$$E = g E_0 + E_1 + g^{-1} E_2 + \cdots. \quad (2.7)$$

Substituting (2.6) - (2.7) into (2.5) and equating the coefficients of $g^{-n}$ on both sides, we find

$$\nabla^2 S_0 = 2v,$$
$$\nabla S_0 \cdot \nabla S_1 = \frac{1}{2} \nabla^2 S_0 - E_0,$$
$$\nabla S_0 \cdot \nabla S_2 = \frac{1}{2} [\nabla^2 S_1 - (\nabla S_1)^2] - E_1,$$
$$\nabla S_0 \cdot \nabla S_3 = \frac{1}{2} [\nabla^2 S_2 - 2 \nabla S_1 \cdot \nabla S_2] - E_2. \quad (2.8)$$
etc. In this way, the second order partial differential equation (2.5) is reduced to a series of first order partial differential equations (2.8). The first of this set of equations can be written as

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

(2.9)

As noted in Ref.[1], 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 (2.8), we note that, in accordance with (2.1) - (2.2) at \(q = 0\), \(\nabla S_0 \propto v^2(0) = 0\). By requiring \(S_1(q)\) to be analytic at \(q = 0\), we determine \(E_0 = \frac{1}{2}(\nabla^2 S_0)_{at \; q=0}. \)  

(2.10)

It is convenient to consider the surface

\[ S_0(q) = \text{constant}; \]  

(2.11)

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

\[ \alpha = (\alpha_1(q), \alpha_2(q), \cdots, \alpha_{N-1}(q)), \]  

(2.12)

so that each \(\alpha\) determines one classical trajectory with

\[ \nabla \alpha_j \cdot \nabla S_0 = 0, \]  

(2.13)

where

\[ j = 1, 2, \cdots, N - 1. \]  

(2.14)

(As an example, we note that as \(q \to 0\), \(v(q) \to \frac{1}{2} \sum_i \omega_i^2 q_i^2\) and therefore \(S_0 \to \frac{1}{2} \sum_i \omega_i q_i^2\). 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 \((q_1, q_2, \cdots, q_N)\) 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 \((q_1, q_2, \cdots, q_N) \to (S_0, \alpha)\) 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 re-
solved by using \((S_0, \alpha)\) as coordinates. Keeping \( \alpha \) fixed, the set of first order partial differential equation can be further reduced to a set of first order ordinary differential equation, which are readily solvable, as we shall see.

Write

\[
S_1(q) = S_1(S_0, \alpha),
\]

the second line of (2.8) becomes

\[
(\nabla S_0)^2 \left( \frac{\partial S_1}{\partial S_0} \right)_{\alpha} = \frac{1}{2} \nabla^2 S_0 - E_0,
\]

and leads to, besides (2.10), also

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

where the integration is taken along the classical trajectory of constant \( \alpha \). Likewise, the third, fourth and other lines of (2.8) lead to

\[
E_1 = \frac{1}{2} [\nabla^2 S_1 - (\nabla S_1)^2] \text{ at } q = 0,
\]

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

\[
E_2 = \frac{1}{2} [\nabla^2 S_2 - 2(\nabla S_1) \cdot (\nabla S_2)] \text{ at } q = 0,
\]

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

etc. These solutions give the convenient normalization convention at \( q = 0 \),

\[
S(0) = 0
\]

and

\[
e^{-S(0)} = 1.
\]
Remarks

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

\[ V(q) = \frac{g^2}{2}(q_1^2 + q_2^2 + \cdots + q_N^2). \] (2.23)

From (2.2), one sees that the Hamilton-Jacobi equation (2.9) is for a particle moving in a potential given by

\[ -v(q) = -\frac{1}{2}(q_1^2 + q_2^2 + \cdots + q_N^2). \] (2.24)

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

\[ S_0(q) = \frac{1}{2}(q_1^2 + q_2^2 + \cdots + q_N^2). \] (2.25)

The corresponding energy is, in accordance with (2.10),

\[ E_0 = \frac{N}{2}. \] (2.26)

By using (2.8), one can readily show that \( E_1 = E_2 = \cdots = 0 \) and \( S_1 = S_2 = \cdots = 0 \). The result is the well-known exact answer with the groundstate wave function for the Schroedinger equation (2.4) given by

\[ e^{-gs(q)} = e^{\frac{-g}{2}(q_1^2 + q_2^2 + \cdots + q_N^2)} \] (2.27)

and the corresponding energy

\[ E = \frac{N}{2}g. \] (2.28)

(ii) From this example, it is clear that the above expression (2.6) - (2.8) is 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.
2.2 Trial Function for the Quantum Double-well Potential

To illustrate how to construct a trial function, consider the quartic potential in one dimension with degenerate minima:

\[ V(x) = \frac{1}{2} g^2 (x^2 - a^2)^2. \]  

(2.29)

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

\[ H = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) \equiv 2gah, \]  

(2.30)

where

\[ h = -\frac{1}{2} \frac{d^2}{dq^2} + \frac{1}{2} q^2 \left( 1 - \frac{q}{\sqrt{8ga^3}} \right)^2. \]  

(2.31)

This shows that the dimensionless (small) expansion parameter is related to \( 1/\sqrt{8ga^3} \); as it turns out, the relevant parameter is its square. In the following, we shall take \( a = 1 \) so that the expansion parameter is \( 1/g \); in the literature[5-14] one often finds the assumption \( 2ga = 1 \) (placing the second minimum of the potential at \( q = 1/g \)) so that \( 1/\sqrt{8ga^3} \) reduces to \( g \) and the anharmonic potential appears as \( (1/2)q^2(1 - qg)^2 \). Then \( g \) appears with positive powers instead of negative, but the coefficients of the power series are the same as with our form of the potential, apart from the overall factor \( 2ga \).

For the above potential (2.29), the Schroedinger equation (2.4) is (with \( a = 1 \))

\[ \left( -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} g^2(x^2 - 1)^2 \right) \psi(x) = E\psi(x) \]  

(2.32)

where, as before, \( \psi(x) = e^{-gS(x)} \) is the groundstate wave function and \( E \) its energy. Using the expansions (2.6) - (2.7) and following the steps (2.8), (2.10) and (2.15) - (2.21), we find the well-known perturbative series

\[ S_0(x) = \frac{1}{3}(x-1)^2(x+2), \quad S_1(x) = \ln \frac{x+1}{2}, \quad S_2(x) = \frac{3}{16} - \frac{x+2}{4(x+1)^2}, \cdots \]  

(2.33)

and

\[ E_0 = 1, \quad E_1 = -\frac{1}{4}, \quad E_2 = -\frac{9}{64}, \cdots. \]  

(2.34)

Both expansions \( S = S_0 + g^{-1}S_1 + g^{-2}S_2 + \cdots \) and \( E = gE_0 + E_1 + g^{-1}E_2 + \cdots \) are divergent, furthermore, at \( x = -1 \) and for \( n \geq 1 \), each \( S_n(x) \) is infinite. The reflection \( x \to -x \) gives a corresponding asymptotic expansion \( S_n(x) \to S_n(-x) \), in which each \( S_n(-x) \) is regular at \( x = -1 \), but singular at \( x = +1 \).
We note that for \( g \) large, the first few terms of the perturbative series (with (2.33) 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 (2.29) 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

\[
\left( \frac{d\phi}{dx} \right)_{x=0} = \phi'(0) = 0. \tag{2.35}
\]

To construct \( \phi(x) \), we start with the first two functions \( S_0(x) \) and \( S_1(x) \) in (2.33). Introduce, for \( x \geq 0 \),

\[
\phi_+(x) \equiv e^{-gS_0(x)-S_1(x)} = \left( \frac{2}{1+x} \right) e^{-gS_0(x)} \tag{2.36}
\]

and

\[
\phi_-(x) \equiv e^{-gS_0(-x)-S_1(x)} = \left( \frac{2}{1+x} \right) e^{-\frac{4}{3}g+S_0(x)}. \tag{2.37}
\]

In order to satisfy (2.35), we define

\[
\phi(x) = \phi(-x) \equiv \begin{cases} \phi_+(x) + \frac{g-1}{g+1} \phi_-(x), & \text{for } 0 \leq x < 1 \\ (1 + \frac{g-1}{g+1} e^{-\frac{4}{3}g}) \phi_+(x), & \text{for } x > 1 \end{cases} \tag{2.38}
\]

Thus, by construct \( \phi'(0) = 0 \), \( \phi(x) \) 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

\[
(T + V + u_+ \phi = g\phi_+ \tag{2.39}
\]

and

\[
(T + V + w) \phi = g\phi, \tag{2.40}
\]

where

\[
u(x) = \frac{1}{(1+x)^2} \tag{2.41}
\]

and

\[w(x) = w(-x) \tag{2.42}\]
with, for \( x \geq 0 \)

\[
w(x) = u(x) + \hat{g}(x) \tag{2.43}
\]

where

\[
\hat{g}(x) = \begin{cases} 
  2g \frac{(g-1)e^{2gS_0(x)} - \frac{4}{3}g}{(g+1)+(g-1)e^{2gS_0(x)}-\frac{4}{3}g^2} & \text{for } 0 \leq x < 1 \\
  0 & \text{for } x > 1.
\end{cases} \tag{2.44}
\]

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, \( w(x) \) also satisfies for \( x > 0 \),

\[
w'(x) < 0, \tag{2.45}
\]

a property that is very useful in our proof of convergence which will be discussed in the next section.
3. Hierarchy Theorem and Its Generalization

In this section, we restrict our discussions to a one-dimensional problem, in which the potential \( V(x) \) is an even function of \( x \), as in the example given in the previous Section 2.2. The Schrödinger equation (1.9) becomes

\[
-\frac{1}{2} \psi''(x) + V(x) \psi(x) = E \psi(x)
\]

with \( \psi(x) \) as its groundstate wave function, \( E \) the groundstate energy and \( ' \) denoting \( \frac{d}{dx} \), as before. For the one-dimensional problem, the trial function \( \phi(x) \) satisfies

\[
-\frac{1}{2} \phi''(x) + U(x) \phi(x) = E_0 \phi(x),
\]

as in (1.11); therefore (3.1) can be written as

\[
-\frac{1}{2} \psi''(x) + (U(x) - E_0) \psi(x) = (w(x) - E) \psi(x),
\]

in which

\[
U(x) = V(x) + w(x)
\]

and

\[
E_0 = E + E,
\]

as before. Throughout this section, we assume

\[
V(x) = V(-x), \quad U(x) = U(-x), \quad \psi(x) = \psi(-x) \quad \text{and} \quad \phi(x) = \phi(-x);
\]

hence, we need only to consider

\[
x \geq 0.
\]

Furthermore, as in the example of the symmetric quartic double-well potential given in Section 2.2, we assume \( w(x) \) to satisfy

\[
w'(x) < 0 \quad \text{for} \quad x > 0
\]

and

\[
w(\infty) = 0.
\]
Therefore, \( w(x) \) is positive for \( x \) positive. Otherwise, the shape of \( w(x) \) can be arbitrary. The Schrödinger equation (3.1) will be solved through the iterative steps (1.34) - (1.43), using the sequences

\[ E_1, E_2, \ldots, E_n, \ldots \] (3.10)

for the energy difference \( E = E_0 - E \), and the sequence

\[ f_1(x), f_2(x), \ldots, f_n(x), \ldots \] (3.11)

for the ratio \( f(x) = \psi(x)/\phi(x) \) with, for \( n = 0 \),

\[ f_0(x) = 1. \] (3.12)

In this section, we differentiate two sets of sequences, labelled \( A \) and \( B \), satisfying different boundary conditions:

\[ f_n(\infty) = 1 \quad \text{for all } n, \quad \text{in Case} \ (A) \]
or

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

Thus, in accordance with (1.42)-(1.43), we have in Case (A)

\[ f_n(x) = 1 - 2 \int_x^\infty \phi^{-2}(y)dy \int_y^\infty \phi^2(z)(w(z) - E_n)f_{n-1}(z)dz, \] (3.13A)

whereas in Case (B)

\[ f_n(x) = 1 - 2 \int_0^x \phi^{-2}(y)dy \int_0^y \phi^2(z)(w(z) - E_n)f_{n-1}(z)dz. \] (3.13B)

In both cases, \( E_n \) is determined by the corresponding \( f_{n-1}(x) \) through (1.38) and (1.40); i.e.,

\[ E_n = [w f_{n-1}]/[f_{n-1}] \] (3.14)

in which \([F]\) of any function \( F(x) \) is defined to be

\[ [F] = \int_0^\infty \phi^2(x)F(x)dx. \] (3.15)

Eqs. (1.35) and (1.37) give

\[ f_n'(x) = -2\phi^{-2}D_n(x). \] (3.16)

Likewise, (1.38) - (1.39) lead to

\[ D_n(x) = -\int_x^\infty \phi^2(z)(w(z) - E_n)f_{n-1}(z)dz \] (3.17)
which, on account of (1.40), is identical to
\[
D_n(x) = \int_0^x \phi^2(z)(w(z) - \mathcal{E}_n)f_{n-1}(z)dz.
\] (3.18)

These two expressions of \(D_n(x)\) are valid for both cases (A) and (B). Let \(x_n\) be defined by
\[
w(x) - \mathcal{E}_n = 0 \quad \text{at} \quad x = x_n.
\] (3.19)

Since \(w'(x) < 0\), (3.19) has one and only one solution, with \(w(x) - \mathcal{E}_n\) negative for \(x > x_n\) and positive for \(x < x_n\). Thus, if
\[
f_{n-1}(x) > 0
\] (3.20)
for all \(x > 0\), we have from (3.17) - (3.18)

\[
D_n(x) > 0
\] (3.21)

and therefore, on account of (3.16),
\[
f'_n(x) < 0.
\] (3.22)

In terms of the electrostatic analog introduced in Section 1, through (1.26) - (1.29), one can form a simple physical picture of these expressions. Represent \(D_n(x)\) by the standard flux of lines of force. Because the dielectric constant \(\kappa(x) = \phi^2(x)\) is zero at \(x = \infty\), so is the displacement field. Hence, \(D_n(\infty) = 0\); therefore each line of force must terminate at a finite point. Since the electric charge density is \(\sigma_n(x) = \phi^2(x)(w(x) - \mathcal{E}_n)f_{n-1}(x)\), the total electric charge to the right of \(x\) is

\[
Q_n(x) = \int_x^\infty \sigma_n(z)dz.
\]

It must also be the negative of the flux \(D_n(x)\) passing through the same point \(x\): i.e.,

\[
D_n(x) = -Q_n(x) = -\int_x^\infty \sigma_n(z)dz,
\]

which gives (3.17). In the whole range from \(x = 0\) to \(\infty\), the total electric charge \(\int_0^\infty \sigma_n(z)dz\) is zero; therefore, we have

\[
Q_n(0) = 0 \quad \text{and} \quad D_n(0) = 0.
\]

Furthermore, at any point \(x > 0\), the total charge from the origin to the point \(x\) is

\[
\int_0^x \sigma_n(z)dz,
\]

which must also be the negative of the above \(Q_n(x)\), and therefore the same as \(D_n(x)\); that leads to (3.18). From (3.19) and \(w'(x) < 0\), one sees that the charge distribution \(\sigma_n(x)\) is
negative for \( x > x_n \), 0 at \( x = x_n \) and positive for \( 0 < x < x_n \). Correspondingly, moving from \( x = \infty \) towards the left, the displacement field increases from \( D_n(\infty) = 0 \) to \( D_n(x) > 0 \), reaching its maximum at \( x = x_n \), then as \( x \) further decreases, so does \( D_n(x) \), and finally reaches \( D_n(0) = 0 \) at \( x = 0 \).

In Case (A), because of \( f_n(\infty) = 1 \), (3.22) leads to

\[
\begin{align*}
f_n(0) &> f_n(x) > f_n(\infty) = 1. 
\end{align*}
\]

Since for \( n = 0 \), \( f_0(x) = 1 \), (3.20) - (3.23A) 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 \( w(x) \).

In Case (B) we assume \( w(x) \) to be not too large, so that (3.13B) is consistent with

\[
f_n(x) > 0 \quad \text{for} \quad x > 0
\]

and therefore

\[
f_n(0) = 1 > f_n(x) > f_n(\infty) > 0. \quad (3.23B)
\]

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 \( n \)

\[
E_{n+1} > E_n \quad (3.24)
\]

and

\[
\frac{d}{dx} \left( \frac{f_{n+1}(x)}{f_n(x)} \right) < 0 \quad \text{at any} \quad x > 0. \quad (3.25)
\]

Thus, the sequences \( \{E_n\} \) and \( \{f_n(x)\} \) are all monotonic, with

\[
E_1 < E_2 < E_3 < \cdots \quad (3.26)
\]

and

\[
1 < f_1(x) < f_2(x) < f_3(x) < \cdots \quad (3.27)
\]

at all finite and positive \( x \).

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

\[
E_1 < E_3 < E_5 < \cdots, \quad (3.28)
\]

but for all even \( n = 2m \), a descending sequence

\[
E_2 > E_4 > E_6 > \cdots; \quad (3.29)
\]

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

$$\mathcal{E}_m > \mathcal{E}_{2l+1}. \quad (3.30)$$

Likewise, at any $x > 0$, for any even $n = 2m$

$$\frac{d}{dx} \left( \frac{f_{2m+1}(x)}{f_{2m}(x)} \right) < 0, \quad (3.31)$$

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

$$\frac{d}{dx} \left( \frac{f_{2l+2}(x)}{f_{2l+1}(x)} \right) > 0. \quad (3.32)$$

Remarks.

1. The validity of Eqs. (3.24) and (3.25) for the boundary condition $f_n(\infty) = 1$ was established in Ref.[4]. The validity of Eqs. (3.28)-(3.32) for the boundary condition $f_n(0) = 1$ is the new result of this paper, which we shall establish.

2. As we shall also show, the lowest eigenvalue $E$ of the Hamiltonian $T + V$ is the limit of the sequence $\{E_n\}$ with

$$E_n = E_0 - \mathcal{E}_n. \quad (3.33)$$

Thus, the boundary condition $f_n(\infty) = 1$ yields a sequence, in accordance with (3.26),

$$E_1 > E_2 > E_3 > \cdots > E, \quad (3.34)$$

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

3. 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 (3.34), with

$$E_1 > E_3 > E_5 > \cdots > E, \quad (3.35)$$

its even members $n = 2m$ satisfy

$$E_2 < E_4 < E_6 < \cdots < E. \quad (3.36)$$

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 $E$.

The proof of the above generalized hierarchy theorem depends on several lemmas that are applicable to both boundary conditions: (A) $f_n(\infty) = 1$ and (B) $f_n(0) = 1$; these lemmas will be established first, and then followed by the proof of the theorem.

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

i) if at all $x > 0$, \( \frac{d}{dx} \left( \frac{f_m(x)}{f_l(x)} \right) < 0 \) then \( \mathcal{E}_{m+1} > \mathcal{E}_{l+1} \), \( (3.37) \)
ii) if at all \( x > 0 \), \( \frac{d}{dx} \left( \frac{f_m(x)}{f_l(x)} \right) > 0 \) then \( \mathcal{E}_{m+1} < \mathcal{E}_{l+1} \). (3.38)

**Proof**

According to (3.14)

\[
\mathcal{E}_{m+1}[f_m] = [w f_m].
\] (3.39)

Also by definition (3.15),

\[
\mathcal{E}_{l+1}[f_m] = [\mathcal{E}_{l+1} f_m].
\] (3.40)

Their difference gives

\[
(\mathcal{E}_{m+1} - \mathcal{E}_{l+1})[f_m] = [(w - \mathcal{E}_{l+1}) f_m].
\] (3.41)

From (3.14),

\[
0 = [(w - \mathcal{E}_{l+1}) f_l].
\] (3.42)

Let \( x_{l+1} \) be defined by (3.19). Multiplying (3.41) by \( f_l(x_{l+1}) \) and (3.42) by \( f_m(x_{l+1}) \) and taking their difference, we have

\[
f_l(x_{l+1})(\mathcal{E}_{m+1} - \mathcal{E}_{l+1})[f_m] = [(w - \mathcal{E}_{l+1})(f_m(x_l)f_l(x_{l+1}) - f_l(x_l)f_m(x_{l+1}))],
\] (3.43)

in which the unsubscripted \( x \) acts as a dummy variable; thus \( [f_m(x)] \) means \( f_m \) and \( [f_m(x_{l+1})] \)

means \( f_m(x_{l+1}) \cdot [1] \), etc.

(i) If \( (f_m(x)/f_l(x))' < 0 \), then for \( x < x_{l+1} \)

\[
\frac{f_m(x)}{f_l(x)} > \frac{f_m(x_{l+1})}{f_l(x_{l+1})}.
\] (3.44)

In addition, since \( w'(x) < 0 \) and \( w(x_{l+1}) = \mathcal{E}_{l+1} \), we also have for \( x < x_{l+1} \)

\[
w(x) > \mathcal{E}_{l+1}.
\] (3.45)

Thus, the function inside the square bracket on the right hand side of (3.43) is positive for \( x < x_{l+1} \). Also, the inequalities (3.44) and (3.45) both reverse their signs for \( x > x_{l+1} \). Consequently, the right hand side of (3.43) is positive definite, and so is its left side. Therefore, on account of (3.23A)-(3.23B), (3.37) holds.

(ii) If \( (f_m(x)/f_l(x))' > 0 \), we see that for \( x < x_{l+1} \), (3.44) reverses its sign but not (3.45). A similar reversal of sign happens for \( x > x_{l+1} \). Thus, the right hand side of (3.43) is now negative definite and therefore \( \mathcal{E}_{m+1} < \mathcal{E}_{l+1} \). Lemma 1 is proved.
The following lemma was already proved in Ref.[4]. For the convenience of the readers, we also include it in this paper. Let

\[ \eta = \eta(\xi) \]  

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

\[ 0 \leq a \leq \xi \leq b \]  

and with

\[ \eta(a) \geq 0. \]

**Lemma 2.**

(i) The ratio \( \eta/\xi \) is a decreasing function of \( \xi \) for \( a < \xi < b \) if

\[ \frac{d\eta}{d\xi} \leq \frac{\eta}{\xi} \quad \text{at} \quad \xi = a \]  

and

\[ \frac{d^2\eta}{d\xi^2} < 0 \quad \text{for} \quad a < \xi < b. \]  

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

\[ \frac{d\eta}{d\xi} \geq \frac{\eta}{\xi} \quad \text{at} \quad \xi = a \]  

and

\[ \frac{d^2\eta}{d\xi^2} > 0 \quad \text{for} \quad a < \xi < b. \]

**Proof** Define

\[ L \equiv \xi \frac{d\eta}{d\xi} - \eta \]  

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

\[ \frac{dL}{d\xi} = \xi \frac{d^2\eta}{d\xi^2} \]  

and

\[ \frac{d}{d\xi} \left( \frac{\eta}{\xi} \right) = \frac{L}{\xi^2}. \]

Since (3.49) says that \( L(a) \leq 0 \) and (3.50) 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 (3.55). The proof of (ii) is the same, but with inequalities reversed.
Lemma 3  For any pair \( f_m(x) \) and \( f_l(x) \)

(i) if over all \( x > 0 \),

\[
\frac{d}{dx} \left( \frac{f_m(x)}{f_l(x)} \right) < 0 \quad \text{then at all } x > 0, \quad \frac{d}{dx} \left( \frac{D_{m+1}(x)}{D_{l+1}(x)} \right) < 0,
\]

and (ii) if over all \( x > 0 \),

\[
\frac{d}{dx} \left( \frac{f_m(x)}{f_l(x)} \right) > 0 \quad \text{then at all } x > 0, \quad \frac{d}{dx} \left( \frac{D_{m+1}(x)}{D_{l+1}(x)} \right) > 0.
\]

Proof  From (3.17)-(3.18), we have

\[
D'_{m+1}(x) = (w(x) - \mathcal{E}_{m+1}) \phi^2(x) f_m(x)
\]

and

\[
D'_{l+1}(x) = (w(x) - \mathcal{E}_{l+1}) \phi^2(x) f_l(x).
\]

Define

\[
\xi = D_{l+1}(x) \quad \text{and} \quad \eta = D_{m+1}(x).
\]

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

Hence, we have

\[
\frac{d\eta}{d\xi} = \frac{D'_{m+1}(x)}{D'_{l+1}(x)} = r(x) \frac{f_m(x)}{f_l(x)}
\]

where

\[
r(x) = \frac{w(x) - \mathcal{E}_{m+1}}{w(x) - \mathcal{E}_{l+1}},
\]

and

\[
\frac{d}{d\xi} \left( \frac{d\eta}{d\xi} \right) = \frac{1}{D'_{l+1}} \left( \frac{D'_{m+1}}{D'_{l+1}} \right)' = \frac{1}{D'_{l+1}} \left( r \frac{f_m}{f_l} \right)'
\]

\[
= \frac{1}{D'_{l+1}} \left( r' \frac{f_m}{f_l} + r \left( \frac{f_m}{f_l} \right)' \right)
\]

where

\[
r'(x) = \frac{\mathcal{E}_{m+1} - \mathcal{E}_{l+1}}{(w(x) - \mathcal{E}_{l+1})^2} w'(x).
\]
(i) If \((f_m/f_l)' < 0\), from Lemma 1, we have

\[ E_{m+1} > E_{l+1}. \]  

(3.65)

From \(w'(x) < 0\) and the definition of \(x_{m+1}\) and \(x_{l+1}\), given by (3.19), we have

\[ x_{m+1} < x_{l+1}, \]  

(3.66)

\[ w(x_{m+1}) = E_{m+1} \quad \text{and} \quad w(x_{l+1}) = E_{l+1}. \]  

(3.67)

We note that from (3.17) - (3.18) \(D_{m+1}(x)\) and \(D_{l+1}(x)\) are both positive continuous functions of \(x\), varying from at \(x = 0\),

\[ D_{m+1}(0) = D_{l+1}(0) = 0 \]  

(3.68)

to at \(x = \infty\)

\[ D_{m+1}(\infty) = D_{l+1}(\infty) = 0 \]  

(3.69)

with their maxima at \(x_{m+1}\) for \(D_{m+1}(x)\) and \(x_{l+1}\) for \(D_{l+1}(x)\), since in accordance with (3.58)-(3.59) and (3.67),

\[ D'_{m+1}(x_{m+1}) = 0 \quad \text{and} \quad D'_{l+1}(x_{l+1}) = 0. \]  

(3.70)

From (3.64)-(3.65), we see that \(r'(x)\) is always \(< 0\). Furthermore, from (3.62), we also find that the function \(r(x)\) has a discontinuity at \(x = x_{l+1}\). At \(x = 0\), \(r(0)\) satisfies

\[ 0 < r(0) = \frac{w(0) - E_{m+1}}{w(0) - E_{l+1}} < 1. \]  

(3.71)

As \(x\) increases from 0, \(r(x)\) decreases from \(r(0)\), through

\[ r(x_{m+1}) = 0, \]  

(3.72)

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

\[ r(\infty) = \frac{E_{m+1}}{E_{l+1}} > 1. \]  

(3.73)

It is convenient to divide the positive \(x\)-axis into three regions:

(I) \(0 < x < x_{m+1}\),

(II) \(x_{m+1} < x < x_{l+1}\)

(III) \(x_{l+1} < x.\)
Table 1. The signs of $D'_{m+1}(x)$, $D'_{l+1}(x)$, $w(x) - E_{m+1}$, $w(x) - E_{l+1}$, $r(x)$ and $r'(x)$ in the three regions defined by (3.74), when $E_{m+1} > E_{l+1}$.

| region | $D'_{m+1}(x)$ | $D'_{l+1}(x)$ | $w(x) - E_{m+1}$ | $w(x) - E_{l+1}$ | $r(x)$ | $r'(x)$ |
|--------|--------------|--------------|-----------------|-----------------|-------|-------|
| I      | $> 0$        | $> 0$        | $> 0$           | $> 0$           | $> 0$ | $< 0$ |
| II     | $< 0$        | $> 0$        | $< 0$           | $> 0$           | $< 0$ | $< 0$ |
| III    | $< 0$        | $< 0$        | $< 0$           | $> 0$           | $< 0$ | $< 0$ |

Table 1 summarizes the signs of $D'_{m+1}$, $D'_{l+1}$, $r$ and $r'$ in these regions. Assuming $(f_m/f_l)' < 0$ we shall show separately the validity of (3.56), $(D_{m+1}/D_{l+1})' < 0$, in each of these three regions.

Since

$$E_{l+1} < w(x) < E_{m+1} \quad \text{in II,}$$

(3.75)

$D_{m+1}(x)$ is decreasing and $D_{l+1}(x)$ is increasing; it is clear that (3.56) holds in II.

In each of regions (I) and (III), we have $r(x) > 0$ from (3.62) and $r'(x) < 0$ from (3.64). Since $(f_m/f_l)'$ is always negative by the assumption in (3.56), both terms inside the big parenthesis of (3.63) are negative; hence the same (3.63) states that $d^2\eta/d\xi^2$ has the opposite sign from $D'_{l+1}$. From the sign of $D'_{l+1}$ listed in Table 1, we see that

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

(3.76)

and

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

(3.77)

Within each region, $\eta = D_{m+1}(x)$ and $\xi = D_{l+1}(x)$ are both monotonic in $x$; therefore, $\eta$ is a single-valued function of $\xi$ and we can apply Lemma 2. In (I), at $x = 0$, both $D_{m+1}(0)$ and $D_{l+1}(0)$ are 0 according to (3.18), but their ratio is given by

$$
\frac{D_{m+1}(0)}{D_{l+1}(0)} = \frac{D'_{m+1}(0)}{D'_{l+1}(0)}.
$$

(3.78)

Therefore,

$$
\left(\frac{d\eta}{d\xi}\right)_{x=0} = \left(\frac{\eta}{\xi}\right)_{x=0}.
$$

(3.79)

Furthermore, from (3.76), $\frac{d^2\eta}{d\xi^2} < 0$ in (I), it follows from Lemma 2, case(i), the ratio $\eta/\xi$ is a decreasing function of $\xi$. Since $\xi' = D'_{l+1}$ is $> 0$ in (I), according to (3.59), we have

$$
\frac{d}{dx}\left(\frac{D_{m+1}}{D_{l+1}}\right) < 0 \quad \text{in (I)}.
$$

(3.80)
In (III), at \( x = \infty \), both \( D_{m+1}(\infty) \) and \( D_{l+1}(\infty) \) are 0 according to (3.69). Their ratio is
\[
\frac{D_{m+1}(\infty)}{D_{l+1}(\infty)} = \frac{D'_{m+1}(\infty)}{D'_{l+1}(\infty)},
\]
which gives at \( x = \infty \),
\[
\left( \frac{d\eta}{d\xi} \right)_{x=\infty} = \left( \frac{\eta}{\xi} \right)_{x=\infty}.
\]

As \( x \) decreases from \( x = \infty \) to \( x = x_{l+1} \), from (3.77) 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 \( \xi' = h'_{l+1} \) is < 0, because \( x > x_{l+1} \), we have
\[
\frac{d}{dx} \left( \frac{D_{m+1}(\xi)}{D_{l+1}(\xi)} \right) < 0 \quad \text{in (III).} \tag{3.82}
\]
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 \( f_{m}(x) \) and \( f_{l}(x) \)

(A) For the boundary condition \( f_{n}(\infty) = 1 \), if at all \( x > 0 \),
\[
\frac{d}{dx} \left( \frac{f_{m}(x)}{f_{l}(x)} \right) < 0 \quad \text{then at all } x > 0, \quad \frac{d}{dx} \left( \frac{f_{m+1}(x)}{f_{l+1}(x)} \right) < 0; \tag{3.83A}
\]
therefore, if at all \( x > 0 \),
\[
\frac{d}{dx} \left( \frac{f_{m}(x)}{f_{l}(x)} \right) > 0 \quad \text{then at all } x > 0, \quad \frac{d}{dx} \left( \frac{f_{m+1}(x)}{f_{l+1}(x)} \right) > 0. \tag{3.84A}
\]

(B) For the boundary condition \( f_{n}(0) = 1 \), if at all \( x > 0 \),
\[
\frac{d}{dx} \left( \frac{f_{m}(x)}{f_{l}(x)} \right) < 0 \quad \text{then at all } x > 0, \quad \frac{d}{dx} \left( \frac{f_{m+1}(x)}{f_{l+1}(x)} \right) > 0; \tag{3.83B}
\]
therefore, if at all \( x > 0 \),
\[
\frac{d}{dx} \left( \frac{f_{m}(x)}{f_{l}(x)} \right) > 0 \quad \text{then at all } x > 0, \quad \frac{d}{dx} \left( \frac{f_{m+1}(x)}{f_{l+1}(x)} \right) < 0. \tag{3.84B}
\]

**Proof** Define
\[
\hat{\xi} = f_{l+1}(x) \quad \text{and} \quad \hat{\eta} = f_{m+1}(x). \tag{3.85}
\]
From (1.35) we see that
\[
\frac{d\hat{\eta}}{d\hat{\xi}} = \frac{f'_{m+1}(x)}{f'_{l+1}(x)} = \frac{D_{m+1}(x)}{D_{l+1}(x)} \tag{3.86}
\]
and

\[
\frac{d}{d\xi} \left( \frac{d\hat{\eta}}{d\xi} \right) = \frac{1}{f_{l+1}'(x)} \frac{d}{dx} \left( \frac{D_{m+1}(x)}{D_{l+1}(x)} \right) .
\] (3.87)

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

\[
\left( \frac{\hat{\eta}}{\hat{\xi}} \right)_{x=\infty} = 1.
\] (3.88)

At the same point \( x = \infty \), in accordance with (3.17), \( D_{l+1}(\infty) = D_{m+1}(\infty) = 0 \), but their ratio is, on account of \( w(\infty) = 0 \) and (3.37) of Lemma 1,

\[
\frac{D_{m+1}(\infty)}{D_{l+1}(\infty)} = \frac{D_{m+1}'(\infty)}{D_{l+1}'(\infty)} = \frac{w(\infty) - \xi_{m+1}}{w(\infty) - \xi_{l+1}} = \frac{\xi_{m+1}}{\xi_{l+1}} > 1,
\] (3.89)

in which the last inequality follows from the same assumption, if \( (f_m/f_l)' < 0 \), shared by (3.37) of Lemma 1 and the present (3.83A) that we wish to prove. Thus, from (3.86), at \( x = \infty \)

\[
\left( \frac{d\hat{\eta}}{d\xi} \right)_{x=\infty} = \frac{\xi_{m+1}}{\xi_{l+1}} > \left( \frac{\hat{\eta}}{\hat{\xi}} \right)_{x=\infty} = 1.
\] (3.90)

As \( x \) decreases from \( \infty \) to 0, \( \hat{\xi} \) increases from \( f_{l+1}(\infty) = 1 \) to \( f_{l+1}(0) > 1 \), in accordance with (3.22) and (3.23A). On account of (3.56) of Lemma 3, we have \( (D_{m+1}/D_{l+1})' < 0 \), which when combined with (3.87) and \( f_{m+1}'(x) < 0 \) leads to

\[
\frac{d}{d\xi} \left( \frac{d\hat{\eta}}{d\xi} \right) > 0.
\] (3.91)

Thus, by using (3.51)-(3.52) of Lemma 2, we have \( \hat{\eta}/\hat{\xi} \) to be an increasing function of \( \hat{\xi} \); i.e.,

\[
\frac{d}{d\xi} \left( \frac{\hat{\eta}}{\hat{\xi}} \right) > 0.
\] (3.92)

Because

\[
\frac{d}{dx} \left( \frac{\hat{\eta}}{\hat{\xi}} \right) = \hat{\xi} \frac{d}{dx} \left( \frac{\hat{\eta}}{\hat{\xi}} \right) = f_{l+1}' \frac{d}{d\xi} \left( \frac{\hat{\eta}}{\hat{\xi}} \right)
\] (3.93)

and \( f_{l+1}' < 0 \), we find

\[
\frac{d}{dx} \left( \frac{f_{m+1}}{f_{l+1}} \right) = \frac{d}{dx} \left( \frac{\hat{\eta}}{\hat{\xi}} \right) < 0,
\] (3.94)
which establishes (3.83A). Through the interchange of the subscripts $m$ and $l$, we also obtain (3.84A).

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

$$\frac{f_{m+1}(0)}{f_{l+1}(0)} = 1. \quad (3.95)$$

Furthermore from (3.16) and (3.18B), we also have $f'_{m+1}(0) = f'_{l+1}(0) = 0$ and $D_{m+1}(0) = D_{l+1}(0) = 0$, with their ratio given by

$$\left(\frac{df_{m+1}}{df_{l+1}}\right)_{x=0} = \frac{f'_{m+1}(0)}{f'_{l+1}(0)} = \frac{D_{m+1}(0)}{D_{l+1}(0)} = \frac{D'_{m+1}(0)}{D'_{l+1}(0)} = \frac{w(0) - \mathcal{E}_{m+1}}{w(0) - \mathcal{E}_{l+1}}. \quad (3.96)$$

From (3.37) of Lemma 1, we see that if $(f_m/f_l)' < 0$, then $\mathcal{E}_{m+1} > \mathcal{E}_{l+1}$ and therefore

$$\left(\frac{df_{m+1}}{df_{l+1}}\right)_{x=0} < 1. \quad (3.97)$$

$$\left(\frac{\hat{\eta}}{\xi}\right)_{x=0} = 1. \quad (3.98)$$

Thus,

$$\left(\frac{d\hat{\eta}}{d\xi}\right)_{x=0} < \left(\frac{\hat{\eta}}{\xi}\right)_{x=0}. \quad (3.99)$$

Analogously to (3.53), define

$$L(x) \equiv \hat{\xi} \frac{d\hat{\eta}}{d\xi} - \hat{\eta} = f_{l+1}(x) \frac{f'_{m+1}(x)}{f'_{l+1}(x)} - f_{m+1}(x); \quad (3.100)$$

therefore

$$\frac{dL(x)}{dx} = \hat{\xi} \frac{dL}{d\xi} = \hat{\xi} \frac{d\hat{\eta}}{d\xi} = \hat{\xi} \frac{d\hat{\eta}}{d\xi} = f_{l+1} \frac{d}{dx} \left(\frac{f'_{m+1}}{f'_{l+1}}\right) = f_{l+1} \frac{d}{dx} \left(\frac{D_{m+1}}{D_{l+1}}\right). \quad (3.101)$$

From (3.56) of Lemma 3, we know that if $(f_m/f_l)' < 0$ then $(D_{m+1}/D_{l+1})' < 0$, which leads to

$$\frac{dL(x)}{dx} < 0. \quad (3.102)$$
From (3.100), we have
\[ L(x) = \hat{\xi} \left( \frac{d\hat{\eta}}{d\xi} - \frac{\hat{\eta}}{\xi} \right) = f_{i+1}(x) \left( \frac{d\hat{\eta}}{d\xi} - \frac{\hat{\eta}}{\xi} \right), \quad (3.103) \]
and therefore at \( x = 0 \), because of (3.99),
\[ L(0) < 0. \quad (3.104) \]
Combining (3.102) and (3.104), we derive
\[ L(x) < 0 \quad \text{for} \quad x \geq 0. \quad (3.105) \]
Multiplying (3.100) by \( f'_{i+1}(x) \), we have
\[ f'_{i+1}(x)L(x) = f_{i+1}(x)f'_{m+1}(x) - f_{m+1}(x)f'_{i+1}(x) \]
\[ = f^2_{i+1}(x) \left( \frac{f_{m+1}(x)}{f_{i+1}(x)} \right)'. \quad (3.106) \]
Because \( f'_{i+1}(x) \) and \( L(x) \) are both negative, it follows then
\[ \left( \frac{f_{m+1}(x)}{f_{i+1}(x)} \right)' > 0, \]
which gives (3.83B) for Case \((B)\), with the boundary condition \( f_n(0) = 1 \). Interchanging the subscripts \( m \) and \( l \), (3.83B) becomes (3.84B), and Lemma 4 is established.

We now turn to the proof of the theorem stated in (3.24)-(3.32).

**Proof of the Hierarchy Theorem**

When \( n = 0 \), we have
\[ f_0(x) = 1. \quad (3.107) \]
From (3.20)-(3.22), we find for \( n = 1 \)
\[ f'_1(x) < 0, \quad (3.108) \]
and therefore
\[ (f_1/f_0)' < 0. \quad (3.109) \]
In Case \((A)\), by using (3.83A) 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, (3.24)-(3.27) are established.
In Case (B), by using (3.109) and (3.83B), and setting $m = 1$ and $l = 0$, we find $(f_2/f_1)' > 0$, which in turn leads to $(f_3/f_2)' < 0$, $\cdots$, and (3.31)-(3.32). Inequalities (3.28)-(3.30) now follow from (3.37)-(3.38) of Lemma 1. The Hierarchy Theorem is proved.

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

$$0 < \mathcal{E}_n < w(0). \quad (3.110)$$

Therefore, each of the monotonic sequences

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

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

and

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

converges to a finite limit $\mathcal{E}$. By following the discussions in Section 5 of Ref.[4], one can show that each of the corresponding monotonic sequences of $f_n(x)$ also converges to a finite limit $f(x)$. The interchange of the limit $n \to \infty$ and the integrations in (3.13A) completes the proof that in Case (A) the limits $\mathcal{E}$ and $f(x)$ satisfy

$$f(x) = 1 - 2 \int_x^\infty \phi^{-2}(y)dy \int_y^\infty \phi^2(z)(w(z) - \mathcal{E})f(z)dz. \quad (3.111A)$$

As noted before, the convergence in Case (A) can hold for any large but finite $w(x)$, provided that $w'(x)$ is negative for $x > 0$. In Case (B), a large $w(x)$ may yield a negative $f_n(x)$, in violation of (3.23B) . Therefore, the convergence does depend on the smallness of $w(x)$. One has to follow discussions similar to those given in Ref.[3] to ensure that the limits $\mathcal{E}$ and $f(x)$ satisfy

$$f(x) = 1 - 2 \int_0^x \phi^{-2}(y)dy \int_0^y \phi^2(z)(w(z) - \mathcal{E})f(z)dz. \quad (3.111B)$$
4. Asymmetric Quartic Double-well Problem

The hierarchy theorem established in the previous section has two restrictions: (i) the limitation of half space $x \geq 0$ and (ii) the requirement of a monotonically decreasing perturbative potential $w(x)$. In this section, we shall remove these two restrictions.

Consider the specific example of an asymmetric quadratic double-well potential

$$V(x) = \frac{1}{2}g^2(x^2 - 1)^2 + g\lambda x$$

with the constant $\lambda > 0$. The groundstate wave function $\psi(x)$ and energy $E$ satisfy the Schrödinger equation

$$(T + V(x))\psi(x) = E\psi(x),$$

where $T = -\frac{d^2}{dx^2}$, as before. In the following, we shall present our method in two steps: We first construct a trial function $\phi(x)$ of the form

$$\phi(x) = \begin{cases} \phi^+(x) & \text{for } x \geq 0 \\ \phi^-(x) & \text{for } x \leq 0 \end{cases}$$

with prime denoting $\frac{d}{dx}$, as before. As we shall see, for $x > 0$, the trial function $\phi(x) = \phi^+(x)$ satisfies

$$(T + V(x) + v_+^+(x))\phi^+(x) = E_0^+ \phi^+(x)$$

with

$$v_+^+(x) < 0,$$  \hspace{1cm} (4.7a)

whereas for $x < 0$, $\phi(x) = \phi^-(x)$ satisfies

$$(T + V(x) + v_-^-\phi^-(x) = E_0^- \phi^-$$

with

$$v_-^-\phi^-(x) > 0.$$  \hspace{1cm} (4.7b)
Furthermore, at $x = \pm \infty$

\[ v_+(\infty) = v_-(-\infty) = 0. \] (4.8)

Starting separately from $\phi^+(x)$ and $\phi^-(x)$ and applying the hierarchy theorem, as we shall show, we can construct from $\phi(x)$ another trial function

\[ \chi(x) = \begin{cases} 
\chi^+(x) & \text{for } x > 0 \\
\chi^-(x) & \text{for } x < 0
\end{cases} \] (4.9)

with $\chi(x)$ and $\chi'(x)$ both continuous at $x = 0$, given by

\[ \chi(0) = \chi^+(0) = \chi^-(0) \] (4.10)

and

\[ \chi'(0) = \chi'^+(0) = \chi'^-(0) = 0. \] (4.11)

In addition, they satisfy the following Schrödinger equations

\[ (T + V(x))\chi^+(x) = E^+\chi^+(x) \quad \text{for } x > 0 \] (4.12)

and

\[ (T + V(x))\chi^-(x) = E^-\chi^-(x) \quad \text{for } x < 0. \] (4.13)

From $V(x)$ given by (4.1) with $\lambda$ positive, we see that at any $x > 0$, $V(x) > V(-x)$; therefore, $E^+ > E^-$. Thus we can use the hierarchy theorem again, and that will lead from $\chi(x)$ to $\psi(x)$, as we shall see.
4.1 Construction of the First Trial Function

We consider first the positive $x$ region. Following Sec. 2.1, we begin with the usual perturbative power series expansion for

$$\psi(x) = e^{-gS(x)} \quad (4.18)$$

with

$$gS(x) = gS_0(+) + S_1(+) + g^{-1}S_2(+) + \cdots \quad (4.19)$$

and

$$E = gE_0(+) + E_1(+) + g^{-1}E_2(+) + \cdots, \quad (4.20)$$

in which $S_n(+) \text{ and } E_n(+) \text{ are } g\text{-independent.}$ Substituting (4.18)-(4.20) into the Schroedinger equation (4.2) and equating both sides, we find

$$S_0'(+) = x^2 - 1, \quad (4.21)$$

$$S_0'(+)S_1'(+) = \frac{1}{2}S_0''(+) + \lambda x - E_0(+), \quad (4.22)$$

etc. Thus, (4.21) leads to

$$S_0(+) = \frac{1}{3}(x - 1)^2(x + 2). \quad (4.23)$$

Since the left side of (4.22) vanishes at $x = 1$, so is the right side; hence, we determine

$$E_0(+) = 1 + \lambda, \quad (4.24)$$

which leads to

$$S_1(+) = (1 + \lambda)\ln(1 + x). \quad (4.25)$$

Of course, the power series expansion (4.19) and (4.20) are both divergent. However, if we retain the first two terms in (4.19), the function

$$\phi(+) = e^{-gS_0(+) - S_1(+) = \left(\frac{1}{1 + x}\right)^{1+\lambda} e^{-gS_0(+)}} \quad (4.26)$$

serves as a reasonable approximation of $\psi(x)$ for $x > 0$, except when $x$ is near zero. By differentiating $\phi(+)$, we find $\phi(+) \text{ satisfies}$

$$(T + V(x) + u_+(x))\phi(+) = gE_0(+\phi(+) \quad (4.27)$$

where

$$u_+(x) = \frac{1}{2} \left(S_1'(+)^2 - S_1''(+)\right) = \frac{(1 + \lambda)(2 + \lambda)}{2(1 + x)^2}. \quad (4.28)$$
In order to construct the trial function $\phi(x)$ that satisfies the boundary condition (4.5), we introduce for $x \geq 0$,

$$\hat{\phi}(+) \equiv \left( \frac{1}{1 + x} \right)^{1+\lambda} e^{-\frac{4}{3}g + gS_0(+)}, \quad (4.29)$$

and

$$\phi^+(x) \equiv \frac{1}{2g} \cdot \left\{ \begin{array}{ll}
(g + 1 + \lambda)\phi(+) + (g - 1 - \lambda)\hat{\phi}(+), & \text{for } 0 < x < 1 \\
((g + 1 + \lambda) + (g - 1 - \lambda)e^{-\frac{4}{3}g})\phi(+), & \text{for } x > 1
\end{array} \right. \quad (4.30)$$

so that $\phi^+(x)$ and its derivative $\phi^{+\prime}(x)$ are both continuous at $x = 1$, and in addition, at $x = 0$ we have $\phi^{+\prime}(0) = 0$. For $x \leq 0$, we observe that $V(x)$ is invariant under

$$\lambda \to -\lambda \quad \text{and} \quad x \to -x. \quad (4.31)$$

The same transformation converts $\phi^+(x)$ for $x$ positive to $\phi^-(x)$ for $x$ negative. Define

$$\phi^-(x) \equiv \frac{1}{2g} \cdot \left\{ \begin{array}{ll}
(g + 1 - \lambda)\phi(-) + (g - 1 + \lambda)\hat{\phi}(-), & \text{for } -1 < x \leq 0 \\
((g + 1 - \lambda) + (g - 1 + \lambda)e^{-\frac{4}{3}g})\phi(-), & \text{for } x < -1
\end{array} \right. \quad (4.32)$$

where

$$\phi(-) = \left( \frac{1}{1 - x} \right)^{1-\lambda} e^{-gS_0(-)}, \quad (4.33)$$

$$\hat{\phi}(-) = \left( \frac{1}{1 - x} \right)^{1-\lambda} e^{-\frac{4}{3}g + gS_0(-)} \quad (4.34)$$

and

$$S_0(-) = \frac{1}{3}(x + 1)^2(-x + 2). \quad (4.35)$$

Both $\phi^-(x)$ and its derivative $\phi^{-\prime}(x)$ are continuous at $x = -1$; furthermore, $\phi^+(x)$ and $\phi^-(x)$ also satisfy the continuity condition (4.4) and (4.5), as well as the Schrödinger equation (4.6a) and (4.6b), with the perturbative potentials $v_+(x)$ and $v_-(x)$ given by

$$v_+(x) = u_+(x) + \hat{g}_+(x) \quad (4.36a)$$

and

$$v_-(x) = u_-(x) + \hat{g}_-(x) \quad (4.36b)$$

in which $u_+(x)$ is given by (4.28),

$$u_-(x) = \frac{(1 - \lambda)(2 - \lambda)}{2(1 - x)^2} \quad (4.37)$$
\[
\hat{g}_+(x) = \begin{cases} 
\frac{2g(1-\lambda)(1+\lambda-x)}{e^{-\frac{4}{3}g} + 2g\delta(0^+)} e^{-\frac{4}{3}g} & \text{for } 0 < x < 1 \\
0 & \text{for } x > 1 
\end{cases} 
\]

and

\[
\hat{g}_-(x) = \begin{cases} 
\frac{2g(1-\lambda)(1+\lambda-x)}{e^{-\frac{4}{3}g} + 2g\delta(0^-)} e^{-\frac{4}{3}g} & \text{for } -1 < x < 0 \\
0 & \text{for } x < -1 
\end{cases} 
\]

In order that \( u_+ \), \( \hat{g}_+ \) be positive for \( x > 0 \) and \( u_- \), \( \hat{g}_- \) positive for \( x < 0 \), we impose

\[ \lambda < 1 \quad \text{and} \quad 1 + \lambda < g, \]

in addition to the earlier condition \( \lambda > 0 \). From (4.28) and (4.37), we have

\[ u'_+(x) = -\frac{(1+\lambda)(2+\lambda)}{(1+x)^3} < 0 \quad \text{for } x > 0 \]

and

\[ u'_-(x) = \frac{(1+\lambda)(2+\lambda)}{(1-x)^3} > 0 \quad \text{for } x < 0. \]

Likewise, from (4.38a) and (4.38b), we find

\[ \hat{g}'_+(x) = \begin{cases} 
-\frac{\lambda}{1+\lambda-x} - \frac{2g(1-x^2)(g+1+\lambda)}{(g+1+\lambda)+(g-1-\lambda) e^{-\frac{4}{3}g} + 2g\delta(0^+)} \hat{g}_+(x) & \text{for } 0 < x < 1 \\
0 & \text{for } x > 1 
\end{cases} \]

and

\[ \hat{g}'_-(x) = \begin{cases} 
-\frac{\lambda}{1-\lambda-x} + \frac{2g(1-x^2)(g+1-\lambda)}{(g+1-\lambda)+(g-1+\lambda) e^{-\frac{4}{3}g} + 2g\delta(0^-)} \hat{g}_-(x) & \text{for } -1 < x < 0 \\
0 & \text{for } x < -1 
\end{cases} \]

Furthermore, as \( x \to \pm 1 \),

\[ \lim_{x \to 1} \hat{g}'_+(x) = -\frac{2g(1-\lambda) e^{-\frac{4}{3}g}}{(g+1+\lambda)+(g-1-\lambda) e^{-\frac{4}{3}g}} \delta(x-1) \]

and

\[ \lim_{x \to -1} \hat{g}'_-(x) = \frac{2g(1+\lambda) e^{-\frac{4}{3}g}}{(g+1-\lambda)+(g-1+\lambda) e^{-\frac{4}{3}g}} \delta(x+1). \]

Thus, for \( x \geq 0 \), we have

\[ g'_+(x) \leq 0 \]
and, together with (4.36a) and (4.40a),

\[ v'_+(x) \leq 0 \]  \tag{4.44a}

for \( x \) positive. On the other hand for \( x \leq 0 \), \( \hat{g}'_-(x) \) is not always positive; e.g., at \( x = 0 \),

\[ \hat{g}'_-(0) = \left( -\frac{\lambda}{1-\lambda} + (g + 1 - \lambda) \right) (1-\lambda)(g-1+\lambda) \]

which is positive for \( g > \frac{3\lambda-1-\lambda^2}{1-\lambda} \), but at \( x = -1+ \),

\[ \hat{g}'_-(1+) = -\lambda \hat{g}_-(-1+) = -\frac{2\lambda g(g-1+\lambda)}{(g+1-\lambda) + (g-1+\lambda)} e^{-\frac{4}{3}g} < 0. \]

However, at \( x = -1 \), \( u'_-(1) = \frac{1}{8}(1+\lambda)(2+\lambda) \). It is easy to see that the sum \( u_- + \hat{g}_- = v_- \) can satisfy for \( x \leq 0 \),

\[ v'_-(x) > 0 \quad \text{if} \quad g \gg 1. \]  \tag{4.44b}

To summarize: \( \phi^+(x) \) and \( \phi^-(x) \) satisfy the Schroedinger equation (4.6a) and (4.6b), with \( v_\pm(x) \) given by (4.36a) and (4.36b),

\[ E^+_0 = gE_0(+) \equiv g(1+\lambda) \]  \tag{4.45a}

and

\[ E^-_0 = gE_0(-) \equiv g(1-\lambda) \]  \tag{4.45b}

and the boundary conditions (4.4) and (4.5). In addition, \( v_\pm(x) \) satisfies

\[ v_+(\infty) = 0, \quad v_-(\infty) = 0 \]  \tag{4.46}

and the monotonicity conditions (4.7a) and (4.7b).
4.2 Construction of the Second Trial Function

To construct the second trial function $\chi(x)$ introduced in (4.9), we define $f^{\pm}(x)$ by

$$
\chi^{+}(x) = \phi^{+}(x)f^{+}(x) \quad \text{for } x \geq 0 \quad (4.47a)
$$

and

$$
\chi^{-}(x) = \phi^{-}(x)f^{-}(x) \quad \text{for } x \leq 0 \quad (4.47b)
$$

To retain flexibility it is convenient to impose only the boundary condition (4.11) first, but not (4.10); i.e., at $x = 0$

$$
\chi^{+}(0) = \chi^{-}(0) = 0, \quad (4.48)
$$

but leaving the choice of the overall normalization of $\chi^{+}(0)$ and $\chi^{-}(0)$ to be decided later. We rewrite the Schrödinger equations (4.12) and (4.13) in their equivalent forms

$$
(T + V(x) + v_{+}(x) - E^{+}_{0})\chi^{+}(x) = (v_{+}(x) - \mathcal{E}^{+})\chi^{+}(x) \quad (4.49a)
$$

and

$$
(T + V(x) + v_{-}(x) - E^{-}_{0})\chi^{-}(x) = (v_{-}(x) - \mathcal{E}^{-})\chi^{-}(x) \quad (4.49b)
$$

where

$$
\mathcal{E}^{+} = E^{+}_{0} - E^{+} \quad (4.50a)
$$

and

$$
\mathcal{E}^{-} = E^{-}_{0} - E^{-}. \quad (4.50b)
$$

Because at $x = 0$, $\phi^{+}(0) = \phi^{-}(0) = 0$, in accordance with (4.5), we have, on account of (4.48),

$$
f^{+}(0) = f^{-}(0) = 0. \quad (4.51)
$$

So far, the overall normalization of $f^{+}(x)$ and $f^{-}(x)$ are still free. We may choose

$$
f^{+}(\infty) = 1 \quad \text{and} \quad f^{-}(-\infty) = 1. \quad (4.52)
$$

From (4.6a), (4.47a), (4.49a) and (4.50a), we see that $f^{+}(x)$ satisfies the integral equation (for $x \geq 0$)

$$
f^{+}(x) = 1 - 2 \int_{x}^{\infty} (\phi^{+}(y))^{-2}dy \int_{y}^{\infty} (\phi^{+}(z))^{2}(v_{+}(z) - \mathcal{E}^{+})f^{+}(z)dz. \quad (4.53a)
$$
Furthermore, from (4.6a) and (4.49a), we also have
\[
\int_{0}^{\infty} (\phi^+(x))^{2}(v_+(x) - \mathcal{E}^+) f^+(x) dx. \tag{4.54a}
\]
Likewise, \(f^-(x)\) satisfies (for \(x \leq 0\))
\[
f^-(x) = 1 - 2 \int_{-\infty}^{x} (\phi^-(y))^{-2} dy \int_{-\infty}^{y} (\phi^-(z))^{2}(v_-(z) - \mathcal{E}^-) f^-(-z) dz \tag{4.53b}
\]
and
\[
\int_{-\infty}^{0} (\phi^-(-x))^{2}(v_-(x) - \mathcal{E}^-) f^-(-x) dx. \tag{4.54b}
\]
The function \(f^+(x)\) and \(f^-(x)\) will be solved through the iterative process described in Section 1. We introduce the sequences \(\{f^\pm_n(x)\}\) and \(\{\mathcal{E}^\pm_n\}\) for \(n = 1, 2, 3, \ldots\), with
\[
f^+_n(x) = 1 - 2 \int_{x}^{\infty} (\phi^+(y))^{-2} dy \int_{y}^{\infty} (\phi^+(z))^{2}(v_+(z) - \mathcal{E}^+_n) f^{+}_{n-1}(z) dz. \tag{4.55a}
\]
for \(x \geq 0\), and
\[
f^-_n(x) = 1 - 2 \int_{-\infty}^{x} (\phi^-(y))^{-2} dy \int_{-\infty}^{y} (\phi^-(z))^{2}(v_-(z) - \mathcal{E}^-_n) f^{-}_{n-1}(z) dz \tag{4.55b}
\]
for \(x \leq 0\), where \(\mathcal{E}^\pm_n\) satisfies
\[
\int_{0}^{\infty} (\phi^+(x))^{2}(v_+(x) - \mathcal{E}^+_n) f^{+}_{n-1}(x) dx \tag{4.56a}
\]
and
\[
\int_{-\infty}^{0} (\phi^-(-x))^{2}(v_-(x) - \mathcal{E}^-_n) f^{-}_{n-1}(x) dx. \tag{4.56b}
\]
Thus, (4.55a) and (4.55b) can also be written in their equivalent expressions
\[
f^+_n(x) = f^+_n(0) - 2 \int_{0}^{x} (\phi^+(y))^{-2} dy \int_{0}^{y} (\phi^+(z))^{2}(v_+(z) - \mathcal{E}^+_n) f^{+}_{n-1}(z) dz. \tag{4.57a}
\]
for \(x \geq 0\), and
\[
f^-_n(x) = f^-_n(0) - 2 \int_{x}^{0} (\phi^-(y))^{-2} dy \int_{y}^{0} (\phi^-(-z))^{2}(v_-(z) - \mathcal{E}^-_n) f^{-}_{n-1}(z) dz \tag{4.57b}
\]
for \(x \leq 0\).
For \( n = 0 \), we set
\[
 f^+_0(x) = f^-_0(x) = 1; \quad (4.58)
\]
through induction and by using (4.55a)-(4.56b), we derive all subsequent \( f^\pm_n(x) \) and \( E^\pm_n \). Because \( v^\pm(x) \) satisfies (4.44a), (4.44b) and (4.46), the Hierarchy theorem proved in Section 3 applies. The boundary conditions \( f^+(\infty) = f^-(\infty) = 1 \), given by (4.52), lead to \( f^+_n(\infty) = f^-_n(\infty) = 1 \), in agreement with (4.55a) and (4.55b). According to (3.24)-(3.27) of Case (A) of the theorem, we have
\[
\begin{align*}
\mathcal{E}_1^+ &< \mathcal{E}_2^+ < \mathcal{E}_3^+ < \cdots, \quad (4.59a) \\
\mathcal{E}_1^- &< \mathcal{E}_2^- < \mathcal{E}_3^- < \cdots, \quad (4.59b) \\
1 &< f^+_1(x) < f^+_2(x) < f^+_3(x) < \cdots \quad (4.60a)
\end{align*}
\]
at all finite and positive \( x \), and
\[
1 < f^-_1(x) < f^-_2(x) < f^-_3(x) < \cdots \quad (4.60b)
\]
at all finite and negative \( x \). Since
\[
\mathcal{E}_n^+ < v^+_0(0) \quad (4.61a)
\]
and
\[
\mathcal{E}_n^- < v^-_0(0) \quad (4.61b)
\]
with both \( v^\pm_0(0) \) finite,
\[
\lim_{n \to \infty} \mathcal{E}_n^+ = \mathcal{E}^+ \quad \text{and} \quad \lim_{n \to \infty} \mathcal{E}_n^- = \mathcal{E}^- \quad (4.62)
\]
both exist. Furthermore, by using the integral equations (4.55a)-(4.55b) for \( f^+_n(x) \) and by following the arguments similar to those given in Section 5 of Ref. 13, we can show that
\[
\lim_{n \to \infty} f^+_n(x) = f^+(x) \quad \text{and} \quad \lim_{n \to \infty} f^-_n(x) = f^-(x) \quad (4.63)
\]
also exist. This leads us from the first trial function \( \phi(x) \) given by (4.3) to \( \phi f^+(x) \) and \( \phi f^-(x) \) which are solutions of
\[
(T + V(x) - E^+) \phi f^+(x) = 0 \quad \text{for } x > 0 \quad (4.64a)
\]
and
\[
(T + V(x) - E^-) \phi f^-(x) = 0 \quad \text{for } x < 0 \quad (4.64b)
\]
with
\[
E^+ = E^+_0 - \mathcal{E}^+ \quad \text{and} \quad E^- = E^-_0 - \mathcal{E}^- \quad (4.65)
\]
and the boundary conditions at \( x = 0 \),
\[
\phi'(0) = f'^+(0) = f'^-(0) = 0. \quad (4.66)
\]
An additional normalization factor multiplying, say, \( f^-(x) \) would enable us to construct the second trial function \( \chi(x) \) that satisfies (4.9)-(4.13).
4.3 Symmetric vs Asymmetric Potential

As we shall discuss, the general description leading from the trial function \( \chi(x) \) to the final wave function \( \psi(x) \) that satisfies the Schrödinger equation (4.2) may be set in a more general framework. Decompose any potential \( V(x) \) into two parts

\[
V(x) \equiv \begin{cases} 
V_a(x), & \text{for } x \geq 0 \\
V_b(x), & \text{for } x \leq 0.
\end{cases}
\] (4.67)

Next, extend the functions \( V_a(x) \) and \( V_b(x) \) by defining

\[
V_a(x) \equiv V_a(-x) \quad \text{for } x < 0
\]
and

\[
V_b(x) \equiv V_b(-x) \quad \text{for } x > 0.
\] (4.68)

Thus, both \( V_a(x) \) and \( V_b(x) \) are symmetric potential covering the entire \( x \)-axis. Let \( \chi_a(x) \) and \( \chi_b(x) \) be the groundstate wave functions of the Hamiltonians \( T + V_a \) and \( T + V_b \):

\[
(T + V_a(x))\chi_a(x) = E_a\chi_a(x)
\] (4.69a)
and

\[
(T + V_b(x))\chi_b(x) = E_b\chi_b(x).
\] (4.69b)

The symmetry (4.68) implies that

\[
\chi_a(x) = \chi_a(-x), \quad \chi_b(x) = \chi_b(-x)
\] (4.70)
and at \( x = 0 \)

\[
\chi'_a(0) = \chi'_b(0) = 0.
\] (4.71)

Choose the relative normalization factors of \( \chi_a \) and \( \chi_b \), so that at \( x = 0 \)

\[
\chi_a(0) = \chi_b(0).
\] (4.72)

The same trial function (4.9) for the specific quartic potential (4.1) is a special example of

\[
\chi(x) \equiv \begin{cases} 
\chi_a(x), & \text{for } x \geq 0 \\
\chi_b(x), & \text{for } x \leq 0
\end{cases}
\] (4.73)

with

\[
\chi_a(x) = \chi^+(x) \quad \text{for } x \geq 0
\]
and

\[
\chi_b(x) = \chi^-(x) \quad \text{for } x \leq 0.
\] (4.74)
In general, from (4.69a)-(4.69b) we see that $\chi(x)$ satisfies

$$(T + V(x) + \hat{w}(x))\chi(x) = \hat{E}_0\chi(x). \quad (4.75)$$

Depending on the relative magnitude of $E_a$ and $E_b$, we define, in the case of $E_a > E_b$

$$\hat{w}(x) = \begin{cases} 
0 & \text{for } x > 0 \\
E_a - E_b & \text{for } x < 0 
\end{cases} \quad (4.76a)$$

and

$$\hat{E}_0 = E_a; \quad (4.77a)$$

otherwise, if $E_b > E_a$, we set

$$\hat{w}(x) = \begin{cases} 
E_b - E_a & \text{for } x > 0 \\
0 & \text{for } x < 0 
\end{cases} \quad (4.76b)$$

and

$$\hat{E}_0 = E_b. \quad (4.77b)$$

Thus, we have either

$$\hat{w}(\infty) = 0 \quad \text{and} \quad \hat{w}'(x) < 0 \quad (4.78a)$$

at all finite $x$, or

$$\hat{w}(-\infty) = 0 \quad \text{and} \quad \hat{w}'(x) > 0 \quad (4.78b)$$

at all finite $x$. A comparison between (4.9)-(4.17) and (4.73)-(4.77a) shows that $w(x)$ of (4.14) and the above $\hat{w}(x)$ differs only by a constant.

As in (4.2), $\psi(x)$ is the groundstate wave function that satisfies

$$(T + V(x))\psi(x) = E\psi(x), \quad (4.79)$$

which can also be written in the same form as (1.14)

$$(T + V(x) + \hat{w}(x) - \hat{E}_0)\psi(x) = (\hat{w}(x) - \hat{E})\psi(x), \quad (4.80)$$

with

$$E = \hat{E}_0 - \hat{E}. \quad (4.81)$$

Here, unlike (1.32), $V(x)$ can now also be asymmetric. Taking the difference between $\psi(x)$ times (4.75) and $\chi(x)$ times (4.80), we derive

$$\int_{-\infty}^{\infty} \chi(x)\psi(x)(\hat{w}(x) - \hat{E})dx = 0. \quad (4.82)$$
Introduce
\[ \psi(x) = \chi(x)f(x), \]
(4.83)
in which \( f(x) \) satisfies
\[ f(x) = f(\infty) - 2 \int_{-\infty}^{x} \chi^{-2}(y)dy \int_{y}^{\infty} \chi^2(z)(\hat{w}(z) - \hat{E})f(z)dz. \]
(4.84)

On account of (4.82)-(4.83), the same equation can also be written as
\[ f(x) = f(-\infty) - 2 \int_{-\infty}^{x} \chi^{-2}(y)dy \int_{-\infty}^{y} \chi^2(z)(\hat{w}(z) - \hat{E})f(z)dz. \]
(4.85)

Eq. (4.80) will again be solved iteratively by introducing
\[ \psi_n(x) = \chi(x)f_n(x) \]
(4.86)
with \( \psi_n \) and its associated energy \( \hat{E}_n \) determined by
\[ (T + V(x) + \hat{w}(x) - \hat{E}_0)\psi_n(x) = (\hat{w}(x) - \hat{E}_n)\psi_{n-1}(x) \]
(4.87)
and
\[ \int_{-\infty}^{\infty} \chi(x)\psi_{n-1}(x)(\hat{w}(x) - \hat{E}_n)dx = 0. \]
(4.88)

In terms of \( f_n(x) \), we have
\[ f_n(x) = f_n(\infty) - 2 \int_{-\infty}^{x} \chi^{-2}(y)dy \int_{y}^{\infty} \chi^2(z)(\hat{w}(z) - \hat{E}_n)f_{n-1}(z)dz. \]
(4.89)

On account of (4.88), we also have
\[ \int_{-\infty}^{\infty} \chi^2(x)(\hat{w}(x) - \hat{E}_n)f_n(x)dx = 0 \]
(4.90)
and
\[ f_n(x) = f_n(-\infty) - 2 \int_{-\infty}^{x} \chi^{-2}(y)dy \int_{-\infty}^{y} \chi^2(z)(\hat{w}(z) - \hat{E}_n)f_{n-1}(z)dz. \]
(4.91)

For definiteness, let us assume that
\[ E_a > E_b \]
(4.92)
in (4.69a)-(4.69b); therefore \( \hat{w}'(x) < 0 \) and \( \hat{w}(\infty) = 0 \), in accordance with (4.76a). Start with, for \( n = 0 \),
\[ f_0(x) = 1, \]
(4.93)
we can derive \( \{ E_n \} \) and \( \{ f_n(x) \} \), with

\[
E_n \equiv \hat{E}_0 - \hat{E}_n, \tag{4.94}
\]

by using the boundary conditions, either

\[
f_n(\infty) = 1 \quad \text{for all } n, \quad (A)
\]

or

\[
f_n(-\infty) = 1 \quad \text{for all } n. \quad (B)
\]

It is straightforward to generalize the Hierarchy theorem to the present case. As in Section 3, in Case (A), the validity of the Hierarchy theorem imposes no condition on the magnitude of \( \hat{w}(x) \). But in Case (B) we assume \( \hat{w}(x) \) to be not too large so that (4.91) and the boundary condition \( f_n(-\infty) = 1 \) is consistent with

\[
f_n(x) > 0 \tag{4.95}
\]

for all finite \( x \). From the Hierarchy theorem, we find in Case (A)

\[
E_1 > E_2 > E_3 > \cdots \tag{4.96}
\]

and

\[
1 \leq f_1(x) \leq f_2(x) \leq f_3(x) \leq \cdots, \tag{4.97}
\]

while in Case (B)

\[
E_1 > E_3 > E_5 > \cdots, \tag{4.98}
\]

\[
E_2 < E_4 < E_6 < \cdots, \tag{4.99}
\]

\[
1 \leq f_1(x) \leq f_3(x) \leq f_5(x) \leq \cdots \tag{4.100}
\]

and

\[
1 \geq f_2(x) \geq f_4(x) \geq f_6(x) \geq \cdots. \tag{4.101}
\]

A soluble model of an asymmetric square-well potential is given in Appendix A to illustrate these properties.
5. The N-Dimensional Problem

The $N$-dimensional case will be discussed in this Section. We begin with the electrostatic analog introduced in Section 1. Suppose that the $(n-1)$th iterative solution $f_{n-1}(q)$ is already known. The $n$th order charge density $\sigma_n(q)$ is

$$\sigma_n(q) = (w(q) - \mathcal{E}_n)\phi^2(q)f_{n-1}(q),$$  \hspace{1cm} (5.1)

in accordance with (1.23)-(1.24). Likewise, from (1.26) and (1.29) the dielectric-constant $\kappa$ of the medium is related to the trial function $\phi(q)$ by

$$\kappa(q) = \phi^2(q),$$ \hspace{1cm} (5.2)

and the $n$th order energy shift $\mathcal{E}_n$ is determined by

$$\int \sigma_n(q)d^Nq = 0.$$ \hspace{1cm} (5.3)

In the following we assume the range of $w(q)$ to be finite, with

$$w(\infty) = 0$$ \hspace{1cm} (5.4)

and

$$0 \leq w(q) \leq W_{\text{max}}.$$ \hspace{1cm} (5.5)

Introduce

$$K(W) \equiv \int \kappa(q)\delta(w(q) - W)d^Nq,$$ \hspace{1cm} (5.6)

where $\delta(w(q) - W)$ is Dirac’s $\delta$-function, $W$ is a constant parameter and the integrations in (5.3) and (5.6) are over all $q$-space. Similarly, for any function $F(q)$, we define

$$F^{\text{av}}(W) \equiv K(W)^{-1}\int F(q)\kappa(q)\delta(w(q) - W)d^Nq.$$ \hspace{1cm} (5.7)

In the $N$-dimensional case, the generalization of $[F]$, introduced by (3.15), is

$$[F] = \int F(q)\phi^2(q)d^Nq.$$ \hspace{1cm} (5.8)

In terms of $F^{\text{av}}(W)$, (5.8) can also be written as

$$[F] = \int_0^{W_{\text{max}}} F^{\text{av}}(W)K(W)dW.$$ \hspace{1cm} (5.9)

Thus from (5.1) and (5.3) we have

$$\mathcal{E}_n = [w(q)f_{n-1}(q)]/[f_{n-1}(q)],$$ \hspace{1cm} (5.10)

the $n$-dimensional extension of (3.14).
Following (1.27)-(1.28), the $n$th order electric field is $-\frac{1}{2}\nabla f_n$ and the displacement field is
\[ D_n = -\frac{1}{2}\kappa \nabla f_n. \]  
(5.11)
The corresponding Maxwell equation is
\[ \nabla \cdot D_n = \sigma_n. \]  
(5.12)
Eqs.(5.11) and (5.12) determine $f_n$ except for an additive constant, which can be chosen by requiring
\[ \text{minimum of } f_n(q) = 1. \]  
(5.13)
Therefore,
\[ f_n(q) \geq 1. \]  
(5.14)
As in the one dimensional case discussed in Section 3, (5.10) gives the same condition of fine energy tuning at each order of iteration. It is this condition that leads to convergent iterative solutions derived in Section 3.

We now conjecture that
\[ \lim_{n \to \infty} \mathcal{E}_n = \mathcal{E} = E_0 - E \]  
(5.15)
and
\[ \lim_{n \to \infty} f_n(q) = f(q) = \psi(q)/\phi(q). \]  
(5.16)
also hold in higher dimensions. Although we are not able to establish this conjecture, in the following we present the proofs of the $N$-dimensional generalizations of some of the lemmas proved in Section 3.

Lemma 1. For any pair $f_m(q)$ and $f_l(q)$ if at all $W$ within the range (5.5),
\[ \frac{d}{dW} \left( \frac{f_m^{av}(W)}{f_l^{av}(W)} \right) > 0, \quad \text{then } \mathcal{E}_{m+1} > \mathcal{E}_{l+1}, \]  
(5.17)
and
\[ \frac{d}{dW} \left( \frac{f_m^{av}(W)}{f_l^{av}(W)} \right) < 0, \quad \text{then } \mathcal{E}_{m+1} < \mathcal{E}_{l+1}. \]  
(5.18)
Proof. For any function $\mathcal{F}(W)$, define
\[ < \mathcal{F}(W) > \equiv \int_0^{W_{\text{max}}} K(W) \mathcal{F}(W) dW, \]  
(5.19)
Thus for any function $F(q)$, we have
\[ [F(q)] = < F^{av}(W) >; \]  
(5.20)
therefore,
\[ \mathcal{E}_n[f_{n-1}(q)] = \mathcal{E}_n < f_{n-1}^{av}(W) > \]  
(5.21)
and
\[ [w(q)f_{n-1}(q)] = \langle W f_{n-1}^a(W) \rangle. \]  
(5.22)

By setting the subscript \( n \) in (5.10) to be \( m + 1 \), we obtain
\[ E_{m+1} < f_m^a(W) >= \langle W f_m^a(W) \rangle. \]  
(5.23)

Also by definition (5.19),
\[ E_{l+1} < f_m^a(W) >= \langle E_{l+1} f_m^a(W) \rangle. \]  
(5.24)

The difference of (5.23) and (5.24) gives
\[ (E_{m+1} - E_{l+1}) < f_m^a(W) >= \langle (W - E_{l+1}) f_m^a(W) \rangle. \]  
(5.25)

From (5.10) and setting the subscript \( n \) to be \( l + 1 \), we have
\[ 0 = \langle (W - E_{l+1}) f_l^a(W) \rangle. \]  
(5.26)

Regard \( f_l^a(E_{l+1}) \) and \( f_m^a(E_{l+1}) \) as two constant parameters. Multiply (5.25) by \( f_l^a(E_{l+1}) \), (5.26) by \( f_m^a(E_{l+1}) \) and take their difference. The result is
\[ (E_{m+1} - E_{l+1}) f_l^a(E_{l+1}) < f_m^a(W) >= \langle (W - E_{l+1}) f_l^a(E_{l+1}) f_m^a(W) - f_l^a(W) f_m^a(E_{l+1}) \rangle, \]  
(5.27)

analogous to (3.43).

(i) If \( \frac{d}{dW}(f_m^a(W)/f_l^a(W)) > 0 \), then for \( W < E_{l+1} \)
\[ \frac{f_m^a(W)}{f_l^a(W)} < \frac{f_m^a(E_{l+1})}{f_l^a(E_{l+1})}. \]  
(5.28)

Thus, the function inside the bracket \(< \) in (5.21) is positive, being the product of two negative factors, \( (W - E_{l+1}) \) and \( (f_l^a(E_{l+1}) f_m^a(W) - f_l^a(W) f_m^a(E_{l+1})) \). Also, when \( W > E_{l+1} \), these two factors both reverse their signs. Consequently (5.17) holds.

(ii) If \( \frac{d}{dW}(f_m^a(W)/f_l^a(W)) < 0 \), we see that for \( W < E_{l+1} \), (5.28) reverses its sign, and therefore the function inside the bracket \(< \) in (5.27) is now negative. The same negative sign can be readily established for \( W > E_{l+1} \). Consequently, (5.18) holds and Lemma 1 is established.

Lemma 2. Identical to Lemma 2 of Section 3.

In order to establish the \( N \)-dimensional generalization of Lemma 3 of Section 3, we define
\[ Q_n(W) \equiv \int_{W}^{W_{max}} dW_1 \int \sigma_n(q) \delta(w(q) - W_1) d^N q. \]  
(5.29)

Because of (5.3), \( Q_n(W) \) is also given by
\[ Q_n(W) = -\int_{0}^{W} dW_1 \int \sigma_n(q) \delta(w(q) - W_1) d^N q. \]  
(5.30)
We may picture that the entire \( q \)-space is divided into two regions

\[ I. \quad w(q) > W \] 

and

\[ II. \quad w(q) < W, \] 

with \( Q_n(W) \) the total charge in \( I \), which is also the negative of the total charge in \( II \). By using (5.1) and (5.7), we see that

\[ -\frac{dQ_n(W)}{dW} = (W - \varepsilon_n) f_{n-1}^{av}(W) K(W). \] 

Lemma 3. For any pair \( f_m(q) \) and \( f_l(q) \) if at all \( W \) within the range (5.5)

(i) \( \frac{d}{dW} \left( \frac{f_m(W)}{f_l^{av}(W)} \right) > 0 \) then \( \frac{d}{dW} \left( \frac{Q_{m+1}(W)}{Q_{l+1}(W)} \right) > 0 \)

(ii) \( \frac{d}{dW} \left( \frac{f_m(W)}{f_l^{av}(W)} \right) < 0 \) then \( \frac{d}{dW} \left( \frac{Q_{m+1}(W)}{Q_{l+1}(W)} \right) < 0. \)

Proof Note that (5.34) and (5.35) are very similar to (3.56) and (3.57). As in (3.60), define

\[ \xi = Q_{l+1}(W) \quad \text{and} \quad \eta = Q_{m+1}(W). \]

From (5.33), we have

\[ -\frac{dQ_{m+1}(W)}{dW} = (W - \varepsilon_{m+1}) f_m(W) K(W). \] 

and

\[ -\frac{dQ_{l+1}(W)}{dW} = (W - \varepsilon_{l+1}) f_l^{av}(W) K(W). \] 

Therefore,

\[ \frac{d\eta}{d\xi} = \frac{dQ_{m+1}(W)}{dW} \frac{dQ_{l+1}(W)}{dW} = r(W) \frac{f_m(W)}{f_l^{av}(W)} \] 

where

\[ r(W) = \frac{W - \varepsilon_{m+1}}{W - \varepsilon_{l+1}}. \]

Furthermore,

\[ \frac{d}{d\xi} \left( \frac{d\eta}{d\xi} \right) = \left( \frac{dQ_{l+1}}{dW} \right)^{-1} \frac{d}{dW} \left( \frac{dQ_{m+1}}{dW} \right) \frac{dQ_{l+1}}{dW} \frac{dQ_{m+1}}{dW} = \left( \frac{dQ_{l+1}}{dW} \right)^{-1} \frac{d}{dW} \left( \frac{f_m}{f_l^{av}} \right) \]

\[ = \left( \frac{dQ_{l+1}}{dW} \right)^{-1} \left( \frac{dr}{dW} \frac{f_m}{f_l^{av}} + r \frac{d}{dW} \left( \frac{f_m}{f_l^{av}} \right) \right), \]

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where
\[
\frac{dr}{dW} = \frac{E_m + 1 - E_l + 1}{(W - E_l + 1)^2},
\]
(5.42)
analogous to (3.61)-(3.64).

According to (5.30), at \( W = 0 \)
\[
Q_{m+1}(0) = Q_{l+1}(0) = 0
\]
(5.43)
and according to (5.29), at \( W = W_{max} \)
\[
Q_{m+1}(W_{max}) = Q_{l+1}(W_{max}) = 0.
\]
(5.44)

From (5.37), we see that the derivative \( \frac{d}{dW} Q_{m+1}(W) \) is positive when \( W < E_{m+1} \), zero at \( W = E_{m+1} \) and negative when \( W > E_{m+1} \). Likewise, from (5.38), \( \frac{d}{dW} Q_{l+1}(W) \) is positive when \( W < E_{l+1} \), zero at \( W = E_{l+1} \) and negative when \( W > E_{l+1} \). Their ratio determines \( \frac{dn}{dξ} \).

(i) If \( \frac{d}{dW}(f_{av}^{m}/f_{av}^{l}) > 0 \), from lemma 1, we have
\[
E_{m+1} > E_{l+1}
\]
(5.45)
and therefore, on account of (5.42)
\[
\frac{dr}{dW} > 0.
\]
(5.46)
At \( W = 0 \),
\[
r(0) = \frac{E_{m+1}}{E_{l+1}} > 1.
\]
(5.47)
As \( W \) increases, so does \( r(W) \). At \( W = E_{l+1} \), \( r(W) \) has a discontinuity, with
\[
r(E_{l+1}+) = \infty
\]
(5.48)
and
\[
r(E_{l+1}+) = -\infty.
\]
(5.49)
As \( W \) increases from \( E_{l+1} \), \( r(W) \) continues to increase, with
\[
r(E_{m+1}) = 0
\]
(5.50)
and
\[
r(W_{max}) = \frac{W_{max} - E_{m+1}}{W_{max} - E_{l+1}} < 1.
\]
(5.51)

It is convenient to divide the range \( 0 < W < W_{max} \) into three regions:

A. \( 0 < W < E_{l+1} \)
(5.52)
B. \( E_{l+1} < W < E_{m+1} \)
(5.53)

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C. \( E_{m+1} < W < W_{\text{max}} \). (5.54)

Assuming \( \frac{d}{dW}(f_m^av/f_{l1}^av) > 0 \), we shall show separately \( \frac{d}{dW}(Q_{m+1}/Q_{l+1}) > 0 \) in these three regions.

In region B, \( Q_{l+1} \) is decreasing, but \( Q_{m+1} \) is increasing. Clearly,

\[
\frac{d}{dW}(Q_{m+1}/Q_{l+1}) > 0. \tag{5.55}
\]

In region A, \( \frac{dQ_{l+1}}{dW} > 0 \), \( r(W) \) is positive according to (5.47)-(5.48) and \( \frac{dr}{dW} \) is always > 0 from (5.46). Therefore from (5.41),

\[
\frac{d^2\eta}{d\xi^2} > 0 \quad \text{in A}. \tag{5.56}
\]

In region C, \( \frac{dQ_{l+1}}{dW} < 0 \), but \( r(W) \) and \( \frac{dr}{dW} \) are both positive. Hence,

\[
\frac{d^2\eta}{d\xi^2} < 0 \quad \text{in C}. \tag{5.57}
\]

Within each region, \( \eta = Q_{m+1}(W) \) and \( \xi = Q_{l+1}(W) \) are both monotonic in \( W \); therefore \( \eta \) is a single-valued function of \( \xi \) and we can apply Lemma 2 of Section 3.

In region A, at \( W = 0 \) both \( Q_{m+1}(0) \) and \( Q_{l+1}(0) \) are 0 according to (5.43), but their ratio is given by

\[
\frac{Q_{m+1}(0)}{Q_{l+1}(0)} = \left( \frac{dQ_{m+1}(W)}{dW} / \frac{dQ_{l+1}(W)}{dW} \right)_{W=0}. \tag{5.58}
\]

Therefore

\[
\left( \frac{d\eta}{d\xi} \right)_{W=0} = \left( \frac{\eta}{\xi} \right)_{W=0}. \tag{5.59}
\]

Furthermore, from (5.56), \( \frac{d^2\eta}{d\xi^2} > 0 \). It follows from Lemma 2 of Section 3, the ratio \( \eta/\xi \) is an increasing function of \( \xi \). Since

\[
\frac{d\xi}{dW} = \frac{dQ_{l+1}(W)}{dW} > 0 \quad \text{in A}, \tag{5.60}
\]

as also have

\[
\frac{d}{dW} \left( \frac{Q_{m+1}}{Q_{l+1}} \right) = \frac{d\xi}{dW} \frac{d}{d\xi} \left( \frac{\eta}{\xi} \right) > 0 \quad \text{in A}. \tag{5.61}
\]

In region C, at \( W = W_{\text{max}} \), both \( Q_{m+1}(W_{\text{max}}) \) and \( Q_{l+1}(W_{\text{max}}) \) are 0 according to (5.44). Their ratio is

\[
\frac{Q_{m+1}(W_{\text{max}})}{Q_{l+1}(W_{\text{max}})} = \left( \frac{dQ_{m+1}(W)}{dW} / \frac{dQ_{l+1}(W)}{dW} \right)_{W=W_{\text{max}}}, \tag{5.62}
\]

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Which gives at $W = W_{\text{max}}$

$$
\left( \frac{d\eta}{d\xi} \right)_{W=W_{\text{max}}} = \left( \frac{\eta}{\xi} \right)_{W=W_{\text{max}}}.
$$

(5.63)

As $W$ decreases from $W_{\text{max}}$ to $E_{m+1}$ in region C, since $E_{m+1} > E_{l+1}$, we have

$$
\frac{d\xi}{dW} = \frac{dQ_{l+1}}{dW} < 0 \quad \text{in } C.
$$

(5.64)

Furthermore, from (5.57), $\frac{d^2\eta}{d\xi^2} < 0$ in region C. It follows from Lemma 2 of Section 3, the ratio $\eta/\xi$ is a decreasing function of $\xi$, which together with (5.64) lead to

$$
\frac{d}{dW} \left( \frac{Q_{m+1}}{Q_{l+1}} \right) > 0 \quad \text{in } C.
$$

(5.65)

Thus, we prove case (i) of Lemma 3. Case (ii) of Lemma 3 follows from case (i) by an exchange of the subscripts $m$ and $l$. Lemma 3 is then proved.

So far, the above Lemmas 1 and 3 are almost identical copies of Lemmas 1 and 3 of Section 3, but now applicable to the $N$-dimensional problem. Difficulty arises when we try to generalize Lemma 4 of Section 3.

It is convenient to transform the Cartesian coordinates $q_1, q_2, \ldots, q_N$ to a new set of orthogonal coordinates:

$$(q_1, q_2, \ldots, q_N) \rightarrow (w(q), \beta_1(q), \ldots, \beta_{N-1}(q))$$

(5.66)

with

$$
\nabla w \cdot \nabla \beta_i = 0
$$

(5.67)

and

$$
\nabla \beta_i \cdot \nabla \beta_j = 0 \quad \text{for } i \neq j,
$$

(5.68)

where $i$ or $j = 1, 2, \ldots, N-1$. Introducing

$$
h_w^2 = 1/(\nabla w)^2, \quad h_i^2 = 1/(\nabla \beta_i)^2
$$

(5.69)

$$
\hat{w} = h_w \nabla w \quad \text{and} \quad \hat{\beta}_i = h_i \nabla \beta_i
$$

(5.70)

In terms of the new coordinates, the components of $D_n$ are

$$(D_n)_w = \hat{w} \cdot D_n \quad \text{and} \quad (D_n)_i = \hat{\beta}_i \cdot D_n.$$  

(5.71)

Its divergence is

$$
\nabla \cdot D_n = (h_w h_\beta)^{-1} \left\{ \frac{\partial}{\partial w} (h_\beta (D_n)_w) + \sum_{i=1}^{N-1} \frac{\partial}{\partial \beta_i} (h_i^{-1} h_w h_\beta (D_n)_i) \right\}.
$$

(5.72)
Combining (5.12) with (5.30), we have

\[ Q_n(W) = - \int_0^W dw \int h_w h_\beta (\nabla \cdot D_n) \prod_{i=1}^{N-1} d\beta_i ; \]  

(5.73)

therefore,

\[ Q_n(W) = - \oint (D_n)_w h_\beta \prod_{i=1}^{N-1} d\beta_i, \]  

(5.74)

in which the integration is along the surface

\[ w(q) = W. \]  

(5.75)

From (5.11) and (5.71), it follows that

\[ (D_n)_w = \frac{1}{2} \kappa \frac{\partial f_n}{\partial w} = - \frac{1}{2} \kappa h_w \nabla w \cdot \nabla f_n. \]  

(5.76)

In terms of curvilinear coordinates, (5.7) can be written as

\[ F^{\text{av}}(W) = K(W)^{-1} \oint F(q) \kappa(q) h_w h_\beta \prod_{i=1}^{N-1} d\beta_i. \]  

(5.77)

Substituting (5.76) into (5.74), we find

\[ Q_n(W) = \frac{1}{2} K(W) (\nabla w \cdot \nabla f_n)^{\text{av}}. \]  

(5.78)

Because \( h_w^{-1} (\partial f_n / \partial w) = \hat{w} \cdot \nabla f_n = h_w (\nabla w \cdot \nabla f_n) \), (5.78) can also be written as

\[ Q_n(W) = \frac{1}{2} K(W) \left( h_w^{-2} \frac{\partial f_n}{\partial w} \right)^{\text{av}}. \]  

(5.79)

Here comes the difficulty. While the above Lemma 3 transfers relations between \( f_m^{\text{av}} / f_l^{\text{av}} \) to those between \( Q_{m+1} / Q_{l+1} \), the latter is

\[ \left( h_w^{-2} \frac{\partial f_{m+1}}{\partial w} \right)^{\text{av}} / \left( h_w^{-2} \frac{\partial f_{l+1}}{\partial w} \right)^{\text{av}} \]  

(5.80)

which is quite different from \( dW f_m^{\text{av}} / dW f_l^{\text{av}} \). This particular generalization of the lemmas in higher dimensions fails to establish the Hierarchy Theorem.

For the one-dimensional case discussed in Section 3, we have \( w' < 0 \) and \( x \geq 0 \); consequently (5.80) is \( f_m^{\text{av}} / f_l^{\text{av}} \). Therefore, Lemma 4 of Section 3 can also be established by using (5.80), and the proof of the Hierarchy Theorem can be completed. 

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Appendix

A.1 A Soluble Example

In this Appendix, we consider a soluble model in which the potential $V(x)$ of (4.67) is

$$V(x) = \begin{cases} 
\infty & \text{for } \gamma < x \\
\frac{1}{2}\mu^2 & \text{for } \alpha < x < \gamma \\
\frac{1}{2}W^2 & \text{for } \alpha < x < \gamma \\
0 & \text{for } -\alpha < x < \alpha \\
\frac{1}{2}W^2 & \text{for } -\gamma < x < -\alpha \\
\infty & \text{for } x < -\gamma,
\end{cases} \quad (A.1)$$

with $W^2 > \mu^2$ and

$$\gamma = \alpha + \beta. \quad (A.2)$$

Following (4.68), we introduce two symmetric potentials:

$$V_a(x) = V_a(-x) \quad \text{and} \quad V_b(x) = V_b(-x) \quad (A.3)$$

with, for $x \geq 0$,

$$V_a(x) = \begin{cases} 
\infty & \text{for } \gamma < x \\
\frac{1}{2}\mu^2 & \text{for } \alpha < x < \gamma \\
\frac{1}{2}W^2 & \text{for } 0 \leq x < \alpha
\end{cases} \quad (A.4)$$

and

$$V_b(x) = \begin{cases} 
\infty & \text{for } \gamma < x \\
0 & \text{for } \alpha < x < \gamma \\
\frac{1}{2}W^2 & \text{for } 0 \leq x < \alpha
\end{cases} \quad (A.5)$$

so that (A.1) can also be written as

$$V(x) = \begin{cases} 
V_a(x) & \text{for } x \geq 0 \\
V_b(x) & \text{for } x \leq 0.
\end{cases} \quad (A.6)$$

Let $\psi(x)$, $\chi_a(x)$ and $\chi_b(x)$ be respectively the groundstate wave functions of

$$(T + V(x))\psi(x) = E\psi(x) \quad (A.7)$$

$$(T + V_a(x))\chi_a(x) = E_a\chi_a(x) \quad (A.8)$$

and

$$(T + V_b(x))\chi_b(x) = E_b\chi_b(x). \quad (A.9)$$

For $|x| > \gamma$, since $V(x) = \infty$, we have

$$\psi(x) = \chi_a(x) = \chi_b(x) = 0.$$
For $|x| < \gamma$, these wave functions are of the form

$$
\psi(x) \propto \begin{cases} 
\sin k (x+\gamma) & \text{for } \alpha < x < \gamma \\
\cosh q(x-\delta) & \text{for } -\alpha < x < \alpha \\
\sin p (x+\gamma) & \text{for } -\gamma < x < -\alpha,
\end{cases}
$$

(A.10)

$$
\chi_a(x) \propto \begin{cases} 
\sin k_a (x+\gamma) & \text{for } \alpha < x < \gamma \\
\cosh q_a x & \text{for } -\alpha < x < \alpha \\
\sin k_a (x+\gamma) & \text{for } -\gamma < x < -\alpha
\end{cases}
$$

(A.11)

and

$$
\chi_b(x) \propto \begin{cases} 
\sin p_b (x+\gamma) & \text{for } \alpha < x < \gamma \\
\cosh q_b x & \text{for } -\alpha < x < \alpha \\
\sin p_b (x+\gamma) & \text{for } -\gamma < x < -\alpha.
\end{cases}
$$

(A.12)

By substituting these solutions to the Schroedinger equations (A.7)-(A.9), we derive

$$
E = \frac{1}{2} p^2 = \frac{1}{2} (W^2 - q^2) = \frac{1}{2} (\mu^2 + k^2),
$$

(A.13)

$$
E_a = \frac{1}{2} (W^2 - q_a^2) = \frac{1}{2} (\mu^2 + k_a^2)
$$

(A.14)

and

$$
E_b = \frac{1}{2} p_b^2 = \frac{1}{2} (W^2 - q_b^2).
$$

(A.15)

The continuity of $\psi'/\psi$ at $x = \pm \alpha$ relates

$$
-k\beta \cot k\beta = q\beta \tanh q (\alpha - \delta)
$$

(A.16)

and

$$
-p\beta \cot p\beta = q\beta \tanh q (\alpha + \delta)
$$

(A.17)

with $\beta$ given by (A.2). In the following, we assume the barrier heights $W$ and $\tilde{W} \equiv (W^2 - \mu^2)^{1/2}$

(A.18)

to be much larger than $k$ and $p$; therefore, the wave function $\psi$ is mostly contained within the two square-wells; i.e., $k\beta$ and $p\beta$ are both near $\pi$. We write

$$
k\beta = \pi - \hat{\theta}, \quad p\beta = \pi - \theta
$$

(A.19)

and expect $\hat{\theta}$ and $\theta$ to be small. Likewise, introduce

$$
k_a\beta = \pi - \hat{\theta}_a, \quad p_b\beta = \pi - \theta_b.
$$

(A.20)
The explicit forms of these angles can be most conveniently derived by recognizing the separate actions of two related small parameters: one proportional to the inverse of the barrier height

\[(W\beta)^{-1} << 1\] (A.21)

and the other

\[e^{-2W\alpha} << 1,\] (A.22)

denoting the much smaller tunnelling coefficient.

To illustrate how these two effects can be separated, let us consider first the determination of \(\theta_b\) given by (A.20). The continuity of \(\chi'/\chi_b\) at \(x = \pm \alpha\) gives

\[-p_b\beta \cot p_b\beta = q_b\beta \tanh q_b\alpha.\] (A.23)

From (A.15), we also have

\[W^2 = p_b^2 + q_b^2.\] (A.24)

Although the two small parameters (A.21) and (A.22) are not independent, their effects can be separated by introducing \(p_\infty\) and \(q_\infty\) that satisfy

\[-p_\infty\beta \cot p_\infty\beta = q_\infty\beta\] (A.25)

and

\[W^2 = p_\infty^2 + q_\infty^2.\] (A.26)

Physically, \(p_\infty\) and \(q_\infty\) are the limiting values of \(p_b\) and \(q_b\) when the distance \(2\alpha\) between the two wells \(\rightarrow \infty\), but keeping the shapes of the two wells unchanged. Hence (A.23) becomes (A.25). Let

\[p_\infty\beta = \pi - \theta_\infty.\] (A.27)

From (A.25), we may expand \(\theta_\infty\) in terms of successive powers of \((W\beta)^{-1}\):

\[\theta_\infty = \frac{\pi}{W\beta} \left(1 - \frac{1}{W\beta} + (1 + \frac{\pi^2}{6})(\frac{1}{W\beta})^2 + O(\frac{1}{W\beta})^3\right)\] (A.28)

which determines both \(p_\infty\) and \(q_\infty\). By substituting

\[\theta_b = \theta_\infty + \nu_1 e^{-2q_\infty\alpha} + O(e^{-4q_\infty\alpha})\] (A.29)

into (A.23) and using (A.24)-(A.28), we determine

\[\nu_1 = \left(\frac{p_\infty q_\infty}{W^2}\right) \frac{2q_\infty\beta}{q_\infty\beta + 1}.\] (A.30)
Likewise, the continuity of $\chi_a'/\chi_a$ at $x = \pm \alpha$ gives

$$-k_a \beta \cot k_a \beta = q_a \beta \tanh k_a \alpha,$$  \hfill (A.31)

with

$$\hat{W}^2 = W^2 - \mu^2 = k_a^2 + q_a^2.$$  \hfill (A.32)

As in (A.25), we introduce $k_\infty$ and $\hat{q}_\infty$ that satisfy

$$-k_\infty \beta \cot k_\infty \beta = \hat{q}_\infty \beta$$  \hfill (A.33)

and

$$\hat{W}^2 = k_\infty^2 + \hat{q}_\infty^2.$$  \hfill (A.34)

Similar to (A.27)-(A.28), we define

$$k_\infty \beta = \pi - \hat{\theta}_\infty.$$  \hfill (A.35)

and derive

$$\hat{\theta}_\infty = \frac{\pi}{W \beta} \left( 1 - \frac{1}{W \beta} + (1 + \frac{\pi}{6}) \left( \frac{1}{W \beta} \right)^2 + O\left( \frac{1}{W \beta}^3 \right) \right).$$  \hfill (A.36)

As in (A.29)-(A.30), we find $\hat{\theta}_a \equiv \pi - k_a \beta$ to be given by

$$\hat{\theta}_a = \hat{\theta}_\infty + \hat{\nu}_1 e^{-2k_\infty \alpha} + O(e^{-4k_\infty \alpha})$$  \hfill (A.37)

with

$$\hat{\nu}_1 = \left( \frac{k_\infty \hat{q}_\infty}{\hat{W}^2} \right) \frac{2\hat{q}_\infty \beta}{\hat{q}_\infty \beta + 1}.$$  \hfill (A.38)

To derive similar expressions for $\theta$ and $\hat{\theta}$ of (A.19), we first note that the transformation

$$\alpha \rightarrow \alpha + \delta$$  \hfill (A.39)

brings (A.23) to (A.17), provided that we also change

$$q_b \rightarrow q, \quad p_b \rightarrow p$$

and therefore

$$\theta_b \rightarrow \theta.$$  \hfill (A.40)

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Since according to (A.1), the asymmetry of $V(x)$ is due to the term $\frac{1}{2}\mu^2 > 0$ in the positive $x$ region, it is easy to see that
\[ \delta > 0, \quad (A.41) \]
as will also be shown explicitly below. Thus, from (A.29) and through the transformations (A.39)-(A.40), we derive
\[ \theta = \theta_\infty + \theta_1 \quad (A.42) \]
where
\[ \theta_1 = \nu_1 e^{-2q_\infty(\alpha+\delta)} + O(e^{-4q_\infty(\alpha+\delta)}) \quad (A.43) \]
with $\nu_1$ given by (A.30). Likewise, we note that the transformation
\[ \alpha \rightarrow \alpha - \delta \quad (A.44) \]
brings (A.31) to (A.16), provided that we also change
\[ k_a \rightarrow k, \quad q_a \rightarrow q \]
and therefore
\[ \hat{\theta}_a \rightarrow \hat{\theta}. \quad (A.45) \]
Here, we must differentiate three different situations:

(i) $\alpha > \delta$, 
(ii) $\alpha = \delta$ \hspace{1cm} (A.46)

and

(iii) $\alpha < \delta$.

In case (i), when
\[ e^{-2q_\infty(\alpha-\delta)} << 1, \quad (A.47) \]
from (A.37) and through the transformations given by (A.44)-(A.45), we find
\[ \hat{\theta} = \hat{\theta}_\infty + \hat{\theta}_1 \quad (A.48) \]
where
\[ \hat{\theta}_1 = \hat{\nu}_1 e^{-2\hat{q}_\infty(\alpha-\delta)} + O(e^{-4\hat{q}_\infty(\alpha-\delta)}) \quad (A.49) \]
with \( \hat{\nu}_1 \) given by (A.38). According to (A.13) and (A.19), we have
\[
\mu^2 \beta^2 = \nu^2 \beta^2 - k^2 \beta^2 = (\pi - \theta)^2 - (\pi - \hat{\theta})^2 \\
= (\pi - \theta_\infty - \theta_1)^2 - (\pi - \hat{\theta}_\infty - \hat{\theta}_1)^2,
\]
which leads to
\[
\mu^2 \beta^2 + (2\pi - \theta_\infty - \hat{\theta}_\infty)(\theta_\infty - \hat{\theta}_\infty) = -2(\pi - \theta_\infty)\theta_1 + 2(\pi - \hat{\theta}_\infty)\hat{\theta}_1 + \theta_1^2 - \hat{\theta}_1^2. \quad (A.50)
\]
Since in accordance from (A.28) and (A.36), we find
\[
\hat{\theta}_\infty - \theta_\infty = \frac{\pi}{\beta} \left( \frac{1}{W} - \frac{1}{W} \right) - \frac{\pi}{\beta^2} \left( \frac{1}{W^2} - \frac{1}{W^2} \right) + \cdots = O \left( \frac{\mu^2 \beta^2}{W^3 \beta^3} \right) \ll \mu^2 \beta^2 \quad (A.52)
\]
and
\[
\theta_\infty + \hat{\theta}_\infty = \frac{\pi}{\beta} \left( \frac{1}{W} + \frac{1}{W} \right) + \cdots \ll 2\pi. \quad (A.53)
\]
Thus, the left side of (A.51) is dominated by its first term, \( \mu^2 \beta^2 \). Since \( \theta_1 \) and \( \hat{\theta}_1 \) are exponentially small, we can neglect \( \theta_1^2 - \hat{\theta}_1^2 \) in (A.51). In addition, because \( \theta_\infty \) and \( \hat{\theta}_\infty \) are much smaller than \( 2\pi \), (A.51) can be reduced to
\[
\mu^2 \beta^2 \approx 2\pi(\hat{\theta}_1 - \theta_1) \approx 2\pi \left( \hat{\nu}_1 e^{-2q_\infty(\alpha - \delta)} - \nu_1 e^{-2q_\infty(\alpha + \delta)} \right) \quad (A.54)
\]
which gives the dependence of \( \delta \) on \( \mu^2 \). It is important to note that an exponentially small \( \mu^2 \) can produce a finite \( \delta \). For \( \delta < \alpha \), at \( x = \delta \) we have, in accordance with (A.10)
\[
\psi'(\delta) = 0, \quad (A.55)
\]
which gives the minimum of \( \psi(x) \). The wave function \( \psi(x) \) has two maxima, one for each potential well.

In case (ii), \( \alpha = \delta \) and (A.16) gives \( \cot k\beta = 0 \), and \( \hat{\theta} \) takes on the critical value \( \hat{\theta}_c \) with
\[
\hat{\theta}_c = \frac{\pi}{2}. \quad (A.56)
\]
In case (iii), \( \hat{\theta} > \frac{\pi}{2} \), \( k\beta < \frac{\pi}{2} \) and \( \psi(x) \) has only one maximum.

As in (4.73) and (4.75) we introduce \( \chi(x) \) through
\[
\chi(x) \equiv \begin{cases} 
\chi_a(x), & \text{for } 0 \leq x \leq \gamma \\
\chi_b(x), & \text{for } -\gamma \leq x \leq 0
\end{cases} \quad (A.57)
\]
so that
\[
(T + V(x) + \hat{w}(x))\chi(x) = \hat{E}_0 \chi(x). \quad (A.58)
\]
in which, same as (4.76a)-(4.77a),
\[
\hat{\psi}(x) = \begin{cases} 
0 & \text{for } 0 < x \leq \gamma \\
E_a - E_b & \text{for } -\gamma \leq x < 0 
\end{cases} \tag{A.59}
\]
and
\[
\hat{E}_0 = E_a \tag{A.60}
\]
with \( E_a \) and \( E_b \) given by (A.14) and (A.15). Since according to (A.4)-(A.5), \( V_a(x) \geq V_b(x) \), we have
\[
E_a > E_b; \tag{A.61}
\]
therefore,
\[
\hat{\psi}'(x) \leq 0. \tag{A.62}
\]
Write the Schroedinger equation (A.7) in the form (4.80):
\[
(T + V(x) + \hat{\psi}(x) - \hat{E}_0)\psi(x) = (\hat{\psi}(x) - \hat{E})\psi(x) \tag{A.63}
\]
with
\[
E = \hat{E}_0 - \hat{E} = E_a - \hat{E}. \tag{A.64}
\]
As in (4.82), we have
\[
\int_{-\gamma}^{\gamma} \chi(x)\psi(x)(\hat{\psi}(x) - \hat{E})dx = 0. \tag{A.65}
\]
In all subsequent equations, we restrict the \( x \)-axis to
\[
|x| \leq \gamma, \tag{A.66}
\]
and set \( \psi(x), \chi(x) \) positive. Define
\[
f(x) = \psi(x)/\chi(x). \tag{A.67}
\]
We have, as in (4.84)-(4.85),
\[
f(x) = f(\gamma) - 2 \int_x^{\gamma} \chi^{-2}(y)dy \int_y^{\gamma} \chi^2(z)(\hat{\psi}(z) - \hat{E})f(z)dz, \tag{A.68}
\]
or, on account of (A.65), the equivalent form
\[
f(x) = f(-\gamma) - 2 \int_{-\gamma}^{x} \chi^{-2}(y)dy \int_{-\gamma}^{y} \chi^2(z)(\hat{\psi}(z) - \hat{E})f(z)dz. \tag{A.69}
\]
The derivation of $f(x)$ is given by

$$f'(x) = -2\chi^{-2}(x)h(x) \tag{A.70}$$

where

$$h(x) = \int_{-\gamma}^{x} \chi^2(z)(\hat{w}(z) - \hat{\mathcal{E}})f(z)dz \tag{A.71}$$

or equivalently,

$$h(x) = -\int_{x}^{\gamma} \chi^2(z)(\hat{w}(z) - \hat{\mathcal{E}})f(z)dz. \tag{A.72}$$

In order to satisfy (A.65) and by using (A.59), we see that

$$(E_a - E_b) > \hat{\mathcal{E}} > 0. \tag{A.73}$$

Thus, (A.71)-(A.73) give

$$h(-\gamma) = h(\gamma) = 0,$$

$$h(x) > 0 \quad \text{for } |x| < \gamma, \tag{A.74}$$

$$h'(x) > 0 \quad \text{for } -\gamma < x < 0$$

and

$$h'(x) < 0 \quad \text{for } 0 < x < \gamma.$$

The positivity of $h(x)$ gives

$$f'(x) < 0 \quad \text{for } |x| < \gamma. \tag{A.75}$$

A.2 A Two-level Model

Before discussing the iterative solutions for $f(x)$ and $\mathcal{E}$, it may be useful to first extract some essential features of the soluble square-well example. Let us first concentrate on Case (i) of (A.46), with the parameters $\alpha$ and $\delta$ satisfying

$$e^{-2q_\infty \alpha} << e^{-2q_\infty (\alpha - \delta)} << 1. \tag{A.76}$$

We shall also neglect $(W\alpha)^{-1}$ or $(W\beta)^{-1}$, when compared to 1. Thus, from (A.27)-(A.28), we have

$$p_\infty \approx \frac{\pi}{\beta}; \tag{A.77}$$

in addition, from(A.30) and (A.38) we find

$$\hat{\nu}_1 \approx \nu_1 \approx \frac{2p_\infty}{W} \approx \frac{2\pi}{W\beta}. \tag{A.78}$$
From (A.54), we have
\[ \frac{1}{2} \mu^2 \simeq \frac{\pi}{\beta^2} \nu_1 e^{-2q_{\infty}(\alpha - \delta)} \simeq \frac{2\pi^2}{W\beta^3} e^{-2q_{\infty}(\alpha - \delta)}. \] (A.79)

On account of (A.15), (A.20), (A.27) and (A.29),
\[ E_b = \frac{1}{2} p_b^2 \simeq \frac{1}{2} (p_{\infty} - \frac{\nu_1}{\beta} e^{-2q_{\infty}\alpha})^2 \] (A.80)
which, for
\[ E_{\infty} = \frac{1}{2} p_{\infty}^2, \] (A.81)
gives
\[ E_b \simeq E_{\infty} - \frac{2p_{\infty}^2}{W\beta} e^{-2q_{\infty}\alpha} \simeq E_{\infty} - \frac{2\pi^2}{W\beta^3} e^{-2q_{\infty}\alpha}. \] (A.82)

On the other hand, from (A.13), (A.19) and (A.42)-(A.43), we see that
\[ E = \frac{1}{2} p^2 \simeq \frac{1}{2} (p_{\infty} - \frac{\nu_1}{\beta} e^{-2q_{\infty}(\alpha + \delta)})^2 \simeq E_{\infty} - \frac{2\pi^2}{W\beta^3} e^{-2q_{\infty}(\alpha + \delta)}. \] (A.83)
Thus, under the condition (A.76), we find
\[ \frac{1}{2} \mu^2 \gg E_{\infty} - E_b \gg E_{\infty} - E. \] (A.84)

As we shall see, these inequalities can be understood in terms of a simple two-level model.

Introduce
\[ \lambda = E_{\infty} - E_b. \] (A.85)

We note that from (A.82),
\[ \lambda \simeq \frac{2\pi^2}{W\beta^3} e^{-2q_{\infty}\alpha}, \] (A.86)
and from (A.79) and (A.83),
\[ \lambda \simeq \frac{1}{2} \mu^2 e^{-2q_{\infty}\delta} \quad \text{and} \quad E_{\infty} - E \simeq \lambda e^{-2q_{\infty}\alpha}. \] (A.87)

Consequently, the three small energy parameters in (A.84) are related by
\[ \frac{1}{2} \mu^2 (E_{\infty} - E) \simeq \lambda^2, \] (A.88)

From \( e^{-2q_{\infty}\delta} << 1 \) and (A.76), we see that
\[ \lambda << \frac{1}{2} \mu^2 << \frac{2\pi^2}{W\beta^3} \] (A.89)
in accordance with (A.79) and (A.84). To understand the role of the parameter $\lambda$, we may start with the definition of $V_b(x)$, given by (A.5), keep the parameters $\beta = \gamma - \alpha$ and $\frac{1}{2}W^2$ fixed, but let the spacing $2\alpha$ between the two potential wells approach $\infty$; in the limit $2\alpha \to \infty$, we have $E_b \to E_\infty$. Thus, $\lambda = E_\infty - E_b$ is the energy shift due to the tunneling between the two potential wells located at $x < -\alpha$ and $x > \alpha$ in $V_b(x)$.

There is an alternative definition for $\lambda$, which may further clarify its physical significance. According to (A.3), $V_b(x)$ is even in $x$; therefore, its eigenstates are either even or odd in $x$. In (A.9), $\chi_b(x)$ is the groundstate of $T + V_b(x)$, and therefore it has to be even in $x$. The corresponding first excited state $\chi_{od}$ is odd in $x$; it satisfies

$$ (T + V_b(x))\chi_{od}(x) = E_{od} \chi_{od}(x). \quad (A.90) $$

We may define $\lambda$ by

$$ 2\lambda \equiv E_{od} - E_b \quad (A.91) $$

and regard (A.85) and (A.86) both as approximate expressions, as we shall see.

Multiplying (A.9) by $\chi_{od}(x)$ and (A.90) by $\chi_b(x)$, then taking their difference we derive

$$ -\frac{1}{2} (\chi_{od}'(x)\chi_b(x) - \chi_b'(x)\chi_{od}(x)) = (E_{od} - E_b)\chi_{od}(x)\chi_b(x). \quad (A.92) $$

From (A.12), we may choose the normalization of $\chi_b$ so that

$$ \chi_b(x) = \chi_b(-x) = \begin{cases} 
\left( \frac{\cosh q_{od} \alpha}{\sin p_{od} \beta} \right) \sin p_b (-x + \gamma) & \text{for } \alpha \leq x \leq \gamma \\
\cosh q_b x & \text{for } 0 \leq x \leq \alpha.
\end{cases} \quad (A.93) $$

Correspondingly,

$$ \chi_{od}(x) = -\chi_{od}(-x) = \begin{cases} 
\left( \frac{\sinh q_{od} \alpha}{\sin p_{od} \beta} \right) \sin p_{od} (-x + \gamma) & \text{for } \alpha \leq x \leq \gamma \\
\sinh q_{od} x & \text{for } 0 \leq x \leq \alpha.
\end{cases} \quad (A.94) $$

with

$$ E_b = \frac{1}{2}p_b^2 \quad \text{and} \quad E_{od} = \frac{1}{2}p_{od}^2. \quad (A.95) $$

As in (A.25) and (A.26), $q_{od}$ and $p_{od}$ are determined by

$$ -p_{od} \beta \cot p_{od} \beta = q_{od} \beta \coth q_{od} \alpha \quad (A.96) $$

and

$$ W^2 = p_{od}^2 + q_{od}^2. \quad (A.97) $$
At $x = 0$, we have
\[
\chi_{od}(0) = 0, \quad \chi_{od}'(0) = q_{od} \quad \text{and} \quad \chi_{b}(0) = 1, \quad \chi_{b}'(0) = 0.
\] (A.98)

Integrating (A.92) from $x = 0$ to $x = \gamma$, we find
\[
\frac{1}{2} q_{od} = (E_{od} - E_{b}) \int_{0}^{\gamma} \chi_{od}(x)\chi_{b}(x)dx.
\] (A.99)

From (A.27)-(A.29), we see that
\[
p_{b}\beta \equiv \pi - \theta_{b} \simeq \pi \quad \text{and} \quad \theta_{b} \simeq \theta_{\infty} \simeq \frac{\pi}{W\beta}.
\] (A.100)

Likewise, we can also show that
\[
p_{od}\beta \equiv \pi - \theta_{od} \simeq \pi \quad \text{and} \quad \theta_{od} \simeq \theta_{\infty} \simeq \frac{\pi}{W\beta}.
\] (A.101)

Thus, $q_{od} \simeq q_{b} \simeq W$, and the integral in (A.99) is
\[
\int_{0}^{\gamma} \chi_{od}(x)\chi_{b}(x)dx \approx \int_{\alpha}^{\gamma} \chi_{od}(x)\chi_{b}(x)dx
\]
\[
= \frac{\sin q_{od}\alpha \cosh q_{b}\alpha}{\sin p_{od}\beta \sin p_{b}\beta} \int_{\alpha}^{\gamma} \sin^{2} p_{\infty}(-x + \gamma)dx
\]
\[
\approx \frac{e^{(q_{od}+q_{b})\alpha}}{4\theta_{od}\theta_{b}} \cdot \frac{1}{2} \beta \approx \frac{W^{2} \beta^{3}}{8\pi^{2}} e^{2q_{\infty}\alpha}.
\] (A.102)

Since $q_{od} \simeq W$, we derive from (A.91)
\[
\lambda \equiv \frac{1}{2}(E_{od} - E_{b}) \approx \frac{2\pi^{2}}{W\beta^{3}} e^{-2q_{\infty}\alpha},
\] (A.103)
in agreement with (A.86).

We are now ready to introduce the two-level model. We shall approximate the Hamiltonian $T + V(x)$, $T + V_{a}(x)$ and $T + V_{b}(x)$ of (A.7)-(A.9) by the following three $2 \times 2$ matrices:
\[
h = E_{\infty} + \begin{pmatrix}
\frac{1}{2}\mu^{2} & -\lambda \\
-\lambda & 0
\end{pmatrix},
\] (A.104)
\[
h_{a} = E_{\infty} + \frac{1}{2}\mu^{2} + \begin{pmatrix}
0 & -\lambda \\
-\lambda & 0
\end{pmatrix}
\] (A.105)
and
\[
h_{b} = E_{\infty} + \begin{pmatrix}
0 & -\lambda \\
-\lambda & 0
\end{pmatrix},
\] (A.106)
with $\psi$, $\chi_a$ and $\chi_b$ as their respective groundstates which satisfy

$$h\psi = E\psi, \quad h_a\chi_a = E_a\chi_a$$

and

$$h_b\chi_b = E_b\chi_b. \quad (A.107)$$

The negative sign in the off-diagonal matrix element $-\lambda$ in (A.104)-(A.106) is chosen to make

$$\chi_a = \chi_b = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (A.108)$$

simulating the evenness of $\chi_a(x)$ and $\chi_b(x)$. Likewise, the analog of $\chi_{od}$ is the excited state of $h_b$, with

$$\chi_{od} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (A.109)$$

and

$$h_b\chi_{od} = E_{od}\chi_{od}. \quad (A.110)$$

It is straightforward to verify that

$$\psi = \begin{pmatrix} \sin \xi \\ \cos \xi \end{pmatrix} \quad (A.111)$$

where

$$\sin 2\xi = \frac{4\lambda}{\sqrt{(4\lambda)^2 + \mu^4}} \quad \text{and} \quad \cos 2\xi = \frac{\mu^2}{\sqrt{(4\lambda)^2 + \mu^4}}. \quad (A.112)$$

$$E = E_\infty + \frac{\mu^2}{4} - \sqrt{\lambda^2 + \left(\frac{\mu^2}{4}\right)^2},$$

$$E_a = E_\infty + \frac{\mu^2}{2} - \lambda \quad (A.113)$$

$$E_b = E_\infty - \lambda$$

and

$$E_{od} = E_\infty + \lambda.$$ 

When $\lambda \ll \frac{\mu^2}{4}$, we have

$$E \approx E_\infty - \frac{2\lambda^2}{\mu^2}, \quad (A.114)$$

in agreement with (A.88).
Next, we wish to examine the relation between the two-level model and the soluble square-well example when $\lambda = O(\mu^2)$. Assume, instead of (A.76),

$$
(W \alpha)^{-1} \ll 1, \quad (W \beta)^{-1} \ll 1, \quad e^{-2q_\infty \alpha} \ll 1
$$

but

$$
e^{-2q_\infty \delta} \sim O(1).
$$

Hence, in the square-well example, (A.83),

$$
E_\infty - E \simeq \frac{2\pi^2}{W\beta^3} e^{-2q_\infty (\alpha + \delta)},
$$

and (A.86),

$$
\lambda \simeq \frac{2\pi^2}{W\beta^3} e^{-2q_\infty \alpha},
$$

remain valid; on the other hand, (A.54) and (A.78) now lead to

$$
\frac{1}{2} \mu^2 \simeq \lambda (e^{2q_\infty \delta} - e^{-2q_\infty \delta}) = 2\lambda \sinh 2q_\infty \delta.
$$

Thus, the above expressions for $E_\infty - E$ and $\lambda$ give

$$
E_\infty - E \simeq \lambda e^{-2q_\infty \delta} = \lambda (\cosh 2q_\infty \delta - \sinh \sinh 2q_\infty \delta)
$$

$$
= \lambda \sqrt{1 + \sinh^2 2q_\infty \delta - \sinh 2q_\infty \delta}.
$$

Together with (A.116), this shows that the soluble square-well example yields

$$
E_\infty - E = \sqrt{\lambda^2 + \left(\frac{\mu^2}{4}\right)^2 - \frac{\mu^2}{4}}
$$

in agreement with (A.113) given by the two-level model.

In both the square-well problem and the simple two-level model, we can also examine the limit, when $\lambda \gg \mu^2$. In that case, (A.113) gives

$$
E = E_\infty - \lambda + \frac{\mu^2}{4} - \frac{1}{32} \frac{\mu^4}{\lambda} + \cdots,
$$

which leads to

$$
E = E_\infty - \lambda = E_b \quad \text{when} \quad \mu^2 = 0,
$$

in agreement with the exact square-well solution. Furthermore, if we include the first order correction in $O(\mu^2)$, (A.115) gives

$$
E \simeq E_\infty + \frac{\mu^2}{4} - \lambda = E_b + \frac{1}{2} (E_a - E_b) + O(\mu^4). \quad (A.117)
$$
As we shall discuss, for the exact square-well solution, (A.117) is also valid. Thus, the simple two-level formula (A.113) may serve as an approximate formula for the exact square-well solution over the entire range of \( \frac{1}{4} \mu^2 / \lambda \).

A.3 Square-well Example (Cont.)

We return to the soluble square-well example discussed in Section A.1. As before, \( \psi(x) \) is the groundstate of \( T + V(x) \) with energy \( E \), which is determined by the Schroedinger equation (A.7). Likewise, \( \chi(x) \) is the trial function given by (A.57); i.e., the groundstate of \( T + V(x) + \hat{w}(x) \) with eigenvalue \( \hat{E}_0 = E_a \), in accordance with (A.58)-(A.60). From (A.59) and (A.65), we see that the energy difference

\[ \hat{E} = E_a - E \]  
(A.118)

satisfies

\[ \hat{E} = \frac{N}{M + N}(E_a - E_b), \]  
(A.119)

where

\[ M = \int_0^\gamma \chi(x) \psi(x) dx \]  
(A.120)

and

\[ N = \int_{-\gamma}^0 \chi(x) \psi(x) dx. \]  
(A.121)

Before we discuss the iterative sequence \( \{ \hat{E}_n \} \) that approaches \( \hat{E} \), as \( n \to \infty \), it may be instructive to verify (A.119) by evaluating the integrals (A.120) and (A.121) directly. Choose the normalization convention of \( \psi \) and \( \chi \) so that at \( x = \gamma \)

\[ \frac{\psi'(\gamma)}{\chi'(\gamma)} = 1. \]  
(A.122)

From (A.10)-(A.12) and (A.57) we write

\[
\psi(x) = \frac{k_a}{k} \left( \frac{\cosh q_a \alpha}{\sin k_a \beta} \right) \begin{cases} 
\sin k \left(-x + \gamma\right) & \text{for} \quad \alpha < x < \gamma \\
\frac{\sin k \beta}{\cosh q(\alpha - \delta)} \cosh q(x - \delta) & \text{for} \quad -\alpha < x < \alpha \\
\frac{\sin k \beta \cosh q(\alpha + \delta)}{\sin p \beta \cosh q(\alpha - \delta)} \sin p \left(x + \gamma\right) & \text{for} \quad -\gamma < x < -\alpha
\end{cases}
\]  
(A.123)

\[
\chi(x) = \begin{cases} 
\frac{\cosh q_a \alpha}{\sin k_a \beta} \sin k_a \left(-x + \gamma\right) & \alpha < x < \gamma \\
\cosh q_a x & \text{for} \quad 0 < x < \alpha \\
\cosh q_b x & \text{for} \quad -\alpha < x < 0 \\
\frac{\cosh q_b \alpha}{\sin p_b \beta} \sin p_b \left(x + \gamma\right) & -\gamma < x < -\alpha.
\end{cases}
\]  
(A.124)
By directly evaluating the integral \( \int \chi(x)\psi(x)dx \), we can readily verify that for \( \gamma \geq x \geq 0 \)
\[
\frac{1}{2}(k^2 - k_a^2) \int_x^\gamma \chi(y)\psi(y)dy = \frac{1}{2}(\chi(x)\psi'(x) - \psi(x)\chi'(x)) \quad \text{(A.125)}
\]
and for \(-\gamma \leq x \leq 0\),
\[
\frac{1}{2}(p^2 - p_b^2) \int_{-\gamma}^x \chi(y)\psi(y)dy = -\frac{1}{2}(\chi(x)\psi'(x) - \psi(x)\chi'(x)). \quad \text{(A.126)}
\]
Both relations can also be inferred from the Schroedinger equations (A.7) and (A.58). Setting \( x = 0 \) and taking the sum (A.125)+(A.126), we derive
\[
\frac{1}{2}(k^2 - k_a^2)M + \frac{1}{2}(p^2 - p_b^2)N = 0
\]
which, on account of (A.13)-(A.18), lead to the expression for the energy shift \( \hat{E} \), in agreement with (A.119).

Next, we proceed to verify directly that \( f(x) = \psi(x)/\chi(x) \) satisfies the integral equation (A.68). With the normalization choice (A.122), we find at \( x = \gamma \), since \( \psi(\gamma) = \chi(\gamma) = 0 \),
\[
f(\gamma) = \frac{\psi'(\gamma)}{\chi'(\gamma)} = 1 , \quad \text{(A.127)}
\]
which gives the constant in the integral equation. The same equation (A.68) can also be cast in an equivalent form:
\[
f(x) = 1 + \int_{-\gamma}^x \chi^{-1}(x)(x|G|z)\chi(z)(\hat{w}(z) - \hat{E})f(z)dz \quad \text{(A.128)}
\]
where \((x|G|z)\) is the Green’s function that satisfies
\[
(T + V(x) + \hat{w}(x) - \hat{E}_0)(x|G|z) = \delta(x - z)
\]
and
\[
(x|G|z) = 0 \quad \text{for} \quad x > z. \quad \text{(A.129)}
\]
For \( x < z \), \((x|G|z)\) is given by
\[
(x|G|z) = -2(\chi(x)\chi(z) - \bar{\chi}(x)\chi(z)) \quad \text{(A.130)}
\]
where
\[
\bar{\chi}(x) \equiv \chi(x) \int_0^x \chi^{-2}(y)dy \quad \text{(A.131)}
\]
is the irregular solution of the same Schrödinger equation (A.58), satisfied by \( \chi(x) \). I.e.,
\[
(T + V(x) + \hat{w}(x))\bar{\chi}(x) = \hat{E}_0\bar{\chi}(x). \quad \text{(A.132)}
\]
Consequently, over the entire range \(-\gamma < x < \gamma\)

\[ \chi'(x)\chi(x) - \chi(x)\chi'(x) = 1. \quad (A.133) \]

According to (A.11), (A.12) and (A.57), we have

\[ \chi(x) = \begin{cases} 
A \sin k_{a}(-x + \gamma) + \frac{1}{k_{a}} \left( \frac{\sin k_{a} \beta}{\cosh q_{a} \alpha} \right) \cos k_{a}(-x + \gamma) & \alpha < x < \gamma \\
\frac{1}{q_{a}} \sinh q_{a}x & 0 < x < \alpha \\
\frac{1}{q_{b}} \sinh q_{b}x & \text{for } -\alpha < x < 0 \\
-B \sin p_{b}(x + \gamma) - \frac{1}{p_{b}} \left( \frac{\sin p_{b} \beta}{\cosh q_{b} \alpha} \right) \cos p_{b}(x + \gamma) & -\gamma < x < -\alpha 
\end{cases} \quad (A.134) \]

where \(A\) and \(B\) are constants given by

\[ A = \frac{1}{q_{a}} \left( \frac{\sinh q_{a} \alpha}{\sin k_{a} \beta} \right) - \frac{1}{k_{a}} \left( \frac{\cos k_{a} \beta}{\cosh q_{a} \alpha} \right) \]

and

\[ B = \frac{1}{q_{b}} \left( \frac{\sinh q_{b} \alpha}{\sin p_{b} \beta} \right) - \frac{1}{p_{b}} \left( \frac{\cos p_{b} \beta}{\cosh q_{b} \alpha} \right). \quad (A.135) \]

Since in (A.128), there are only single integrations of the products \(\chi(z)\psi(z)\) and \(\overline{\chi(z)}\psi(z)\), one can readily verify that \(f(x)\) satisfies the integral equation, and therefore also its equivalent form (A.68).

**A.4 The Iterative Sequence**

The integral equation (A.68), or its equivalent form (A.128), will now be solved iteratively by introducing

\[ \psi_{n}(x) = \chi(x)f_{n}(x). \quad (A.136) \]

As in (4.87)-(4.89), \(f_{n}(x)\) and its associated energy \(\hat{\mathcal{E}}_{n}\) are determined by

\[ f_{n}(x) = 1 - 2 \int_{x}^{1} \chi^{-2}(y)dy \int_{y}^{1} \chi^{2}(z)(\hat{w}(z) - \hat{\mathcal{E}}_{n})f_{n-1}(z)dz \quad (A.137) \]

and

\[ \int_{-\gamma}^{\gamma} \chi^{2}(z)(\hat{w}(z) - \hat{\mathcal{E}}_{n})f_{n-1}(z)dz = 0. \quad (A.138) \]

When \(n = 0\), we set

\[ f_{0}(x) = 1. \quad (A.139) \]

Introduce

\[ M_{n} \equiv \int_{0}^{1} \chi^{2}(x)f_{n}(x)dx \quad (A.140) \]

and

\[ N_{n} \equiv \int_{-\gamma}^{0} \chi^{2}(x)f_{n}(x)dx. \quad (A.141) \]
From (A.59) and
\[ E_n \equiv E_a - \hat{E}_n, \quad (A.141) \]
we derive
\[ \hat{E}_n = \frac{N_{n-1}}{M_{n-1} + N_{n-1}}(E_a - E_b) \quad (A.142) \]
and
\[ E_n = \frac{M_{n-1}E_a + N_{n-1}E_b}{M_{n-1} + N_{n-1}}. \quad (A.143) \]

For \( n = 1 \), we have from (A.139)-(A.141),
\[ M_0 = \frac{1}{2} \left\{ \alpha + \frac{1}{2q_a} \sinh 2q_a \alpha + \frac{\cosh^2 q_a \alpha}{\sin^2 k_a \beta} (\beta - \frac{1}{2k_a} \sin 2k_a \beta) \right\}, \quad (A.144) \]
\[ N_0 = \frac{1}{2} \left\{ \alpha + \frac{1}{2q_b} \sinh 2q_b \alpha + \frac{\cosh^2 q_b \alpha}{\sin^2 p_b \beta} (\beta - \frac{1}{2p_b} \sin 2p_b \beta) \right\} \quad (A.145) \]
and
\[ E_1 = E_b + \frac{M_0}{M_0 + N_0}(E_a - E_b). \quad (A.146) \]

For small \( \mu^2 \), since \( E_a - E_b \) and \( M_0 - N_0 \) are both \( O(\mu^2) \), we find
\[ E_1 \approx E_b + \frac{1}{2}(E_a - E_b) + O(\mu^4) \quad (A.147) \]
in agreement with (A.117), given by the simple two-level formula.

Next, we examine the integration for \( f_n(x) \). Consider first the region
\[ \alpha < x < \gamma; \quad (A.148) \]
(A.137) can be written as
\[ f_n(x) = 1 + 2\hat{E}_n \int_x^\gamma \chi^{-2}(y) dy \int_y^\gamma \chi^2(z) f_{n-1}(z) dz. \quad (A.149) \]

Introduce
\[ \xi = k_a(-x + \gamma) \quad (A.150) \]
\[ \epsilon_m = \frac{2\hat{E}_m}{k_a^2} \quad (A.151) \]
and
\[ \psi_n(x) = \chi(x) f_n(x) = \left\{ \begin{array}{l} \cosh q_a \alpha \\ \sin k_a \beta \end{array} \right\} v_n(\xi). \quad (A.152) \]

When \( n = 0 \), we set
\[ v_0(\xi) = \sin \xi. \quad (A.153) \]
From (A.149), or more conveniently by using \((x|G|z)\) given by (A.130), one can readily verify that, for \(\alpha < x < \gamma\),

\[
\begin{align*}
v_1(\xi) &= (1 + \frac{1}{2} \epsilon_1) \sin \xi - \frac{1}{2} \epsilon_1 \xi \cos \xi, \\
v_2(\xi) &= \left\{ (1 + \frac{1}{2} \epsilon_2 + \frac{3}{8} \epsilon_1 \epsilon_2) - \frac{1}{8} \epsilon_1 \epsilon_2 \xi^2 \right\} \sin \xi - (\frac{1}{2} \epsilon_2 + \frac{3}{8} \epsilon_1 \epsilon_2) \xi \cos \xi, \quad (A.154) \\
v_3(\xi) &= \left\{ (1 + \frac{1}{2} \epsilon_3 + \frac{3}{8} \epsilon_2 \epsilon_3 + \frac{5}{16} \epsilon_1 \epsilon_2 \epsilon_3) - \frac{1}{8} (\epsilon_2 \epsilon_3 + \epsilon_1 \epsilon_2 \epsilon_3) \xi^2 \right\} \sin \xi \\
& \quad + \left\{ -(\frac{1}{2} \epsilon_2 + \frac{3}{8} \epsilon_2 \epsilon_3 + \frac{5}{16} \epsilon_1 \epsilon_2 \epsilon_3) \xi + \frac{1}{48} \epsilon_1 \epsilon_2 \epsilon_3 \xi^3 \right\} \cos \xi,
\end{align*}
\]

etc. These solutions can also be readily derived by directly using the differential equation satisfied by \(\psi_n(x) = \chi(x) f_n(x)\):

\[
(T + V(x) + \hat{\omega}(x) - E_a) \psi_n(x) = (\hat{\omega}(x) - \hat{\mathcal{E}}_n) \psi_{n-1}(x), \quad (A.155)
\]

where in accordance with (A.14), \(E_a = \frac{1}{2} (\mu^2 + k_a^2)\). For \(\alpha < x < \gamma\), we have

\[
V(x) = \frac{1}{2} \mu^2, \quad \hat{\omega}(x) = 0
\]

and therefore

\[
(T - \frac{1}{2} k_a^2) \psi_n(x) = -\hat{\mathcal{E}}_n \psi_{n-1}(x). \quad (A.156)
\]

Introduce \(S_n(\xi)\) and \(C_n(\xi)\) to be polynomials in \(\xi\), with

\[
v_n(\xi) \equiv \left( \prod_{m=1}^{n} \epsilon_m \right) \{S_n(\xi) \sin \xi + C_n(\xi) \cos \xi \}. \quad (A.157)
\]

From (A.152) and (A.156)-(A.157), we find

\[
\ddot{S}_n(\xi) - 2 \dot{C}_n(\xi) = S_{n-1}(\xi) \quad (A.158)
\]

and

\[
\ddot{C}_n(\xi) + 2 \dot{S}_n(\xi) = C_{n-1}(\xi),
\]

where the dot denotes \(\frac{d}{d\xi}\), so that \(\dot{S}_n = \frac{dS_n}{d\xi}\), etc. At \(x = \gamma\), we have \(\xi = 0\), \(f_n(\gamma) = \psi'_n(\gamma)/\chi'(\gamma) = 1\) and therefore

\[
S_n(0) + \dot{C}_n(0) = \prod_{m=1}^{n} \epsilon_m^{-1}. \quad (A.159)
\]

For \(n = 0\), \(S_0(\xi) = 1\) and \(C_0(\xi) = 0\). Therefore, for \(n = 1\), (A.158) becomes

\[
\begin{align*}
\ddot{S}_1 &= 1 \\
\ddot{C}_1 &= 0.
\end{align*} \quad (A.160)
\]
Assuming $S_1$ and $C_1$ to be both polynomials of $\xi$, we can readily verify that $S_1$ is a constant and $C_1$ is proportional to $\xi$. Using (A.160) and the boundary condition (A.159), we can establish the first equation in (A.154), and likewise the other equations for $n > 1$.

To understand the structure of $v_1(\xi)$, $v_2(\xi)$, $v_3(\xi)$, \ldots, we may turn to the exact solution $\psi(x)$ given by (A.123). In analogy to (A.152), we define $v(\xi)$ through

$$
\psi(x) \equiv \cosh q_a \alpha \over \sin k_a \beta v(\xi) .
$$

(A.161)

Thus, for $\alpha < x < \gamma$,

$$
v(\xi) = \frac{k_a}{k} \sin k(-x + \gamma).
$$

(A.162)

From (A.13)-(A.14) and (A.118), we have

$$
\hat{E} = E_a - E = \frac{1}{2} (k_a^2 - k^2).
$$

(A.163)

In terms of

$$
\epsilon \equiv \frac{2\hat{E}}{k_a^2} = 1 - \frac{k^2}{k_a^2} ,
$$

(A.164)

we write

$$
v(\xi) = \frac{1}{\sqrt{1 - \epsilon}} \sin(\xi \sqrt{1 - \epsilon})
$$

(A.165)

with $\xi$ given by (A.150), as before. It is straightforward to expand $v(\xi)$ as a power series in $\epsilon$:

$$
v(\xi) = \left\{ \left( 1 + \frac{1}{2} \epsilon + \frac{3}{8} \epsilon^2 + \frac{5}{16} \epsilon^3 \right) - \frac{1}{8} (\epsilon^2 + \epsilon^3) \xi^2 \right\} \sin \xi
$$

$$
+ \left\{ -\left( \frac{1}{2} \epsilon + \frac{3}{8} \epsilon^2 + \frac{5}{16} \epsilon^3 \right) \xi + \frac{1}{48} \epsilon^3 \xi^3 \right\} \cos \xi + O(\epsilon^4)
$$

(A.166)

To compare the above series with $v_n(\xi)$ of (A.154), we can neglect $O(\epsilon^{n+1})$ in (A.166). The replacements of all linear $\epsilon$-terms by $\epsilon_n$, $\epsilon^2$-terms by $\epsilon_{n-1} \epsilon_n$, $\epsilon^3$-terms by $\epsilon_{n-2} \epsilon_{n-1} \epsilon_n$, etc. lead from (A.166) to $v_n(\xi)$. It is of interest to note that the expansion (A.166) of $v(\xi)$ in power of $\epsilon$ has a radius of convergence

$$
|\epsilon| < 1.
$$

(A.167)

On the other hand, the iterative sequence $\{v_n(\xi)\}$ is always convergent, on account of the Hierarchy Theorem. The main difference between (A.154) and (A.166) is that in (A.154) each iterative $\epsilon_n$ is determined by the fraction (A.142).
When the constant $\kappa$ is determined by requiring $\psi_1(x)$ and $\psi'_1(x)$ to be continuous at $x = \alpha$. In region I, when $x = \alpha+$, we have
\[
\psi_1(\alpha+) = \frac{\cosh q_{a\alpha}}{\sin k_{a\beta}} \left\{ (1 + \frac{1}{2} \epsilon_1) \sin k_{a\beta} - \frac{1}{2} \epsilon_1 k_{a\beta} \cos k_{a\beta} \right\} 
\]
and
\[
\psi'_1(\alpha+) = -k_a \frac{\cosh q_{a\alpha}}{\sin k_{a\beta}} \left\{ \cos k_{a\beta} + \frac{1}{2} \epsilon_1 k_{a\beta} \sin k_{a\beta} \right\} 
\]
where the constant
\[
\epsilon_1 = \frac{2}{k_a^2} (E_a - E_1) = \epsilon_1(x) \quad \text{in I} \quad (A.170)
\]
with
\[
E_1 = E_a - \hat{\xi}_1. 
\]
In region II, when $x = \alpha$–
\[
\psi_1(\alpha-) = (k_{II} + \frac{1}{2} \epsilon_{II} q_{a\alpha}) \sinh q_{a\alpha} + \rho_{II} \cosh q_{a\alpha} 
\]
and
\[
\psi'_1(\alpha-) = q_a \left\{ (k_{II} + \frac{1}{2} \epsilon_{II} q_{a\alpha}) \cosh q_{a\alpha} + (\rho_{II} + \frac{1}{2} \epsilon_{II}) \sinh q_{a\alpha} \right\} 
\]
where the constant
\[
\epsilon_{II} = \frac{2}{q_a^2} (E_a - E_1) = \epsilon_1(x) \quad \text{in II}. 
\]
The constants $\kappa_{II}$ and $\rho_{II}$ are determined by
\[
\psi_1(\alpha-) = \psi_1(\alpha+) \quad \text{and} \quad \psi'_1(\alpha-) = \psi'_1(\alpha+). 
\]
Likewise, the constants $\kappa_{III}$ and $\rho_{III}$ are given by
\[
\psi_1(0-) = \psi_1(0+) \quad \text{and} \quad \psi'_1(0-) = \psi'_1(0+), 
\]
and the constants $\kappa_{IV}$ and $E_1$ are determined by
\[
\psi_1(-\alpha-) = \psi_1(-\alpha+) \quad \text{and} \quad \psi'_1(-\alpha-) = \psi'_1(-\alpha+). 
\]

Table 2. The $n = 1$ iterative solution $\psi_1(x)$ in the four regions:

| region | $\epsilon_1(x)$ | $\xi(x)$ | $\psi_1(x)$ |
|--------|----------------|----------|-------------|
| I      | $\frac{\alpha}{k_a^2} (E_a - E_1)$ | $k_a(-x + \gamma)$ | $\cosh q_{a\alpha} \left\{ (1 + \frac{1}{2} \epsilon_1) \sin \xi - \frac{1}{2} \epsilon_1 \xi \cos \xi \right\} \frac{\sin k_{a\beta}}{\sin k_{a\beta}}$ |
| II     | $\frac{\alpha}{q_a^2} (E_a - E_1)$ | $q_{a}x$ | $(\kappa_{II} + \frac{1}{2} \epsilon_{II} \xi) \sinh \xi + \rho_{II} \cosh \xi$ |
| III    | $-\frac{\alpha}{q_a^2} (E_b - E_1)$ | $-q_{b}x$ | $(\kappa_{III} + \frac{1}{2} \epsilon_{III} \xi) \sinh \xi + \rho_{III} \cosh \xi$ |
| IV     | $\frac{\alpha}{q_b^2} (E_b - E_1)$ | $p_{b}(x + \gamma)$ | $\cosh q_{a\alpha} \left\{ (1 + \frac{1}{2} \epsilon_1) \sin \xi - \frac{1}{2} \epsilon_1 \xi \cos \xi \right\} \frac{\sin k_{b\beta}}{\sin k_{b\beta}}$ |

The results for $n = 1$ are given in Table 2. The functions $\psi_1(x)$ and $\xi(x)$ are discontinuous from region to region. The constants $\kappa_{II}$ and $\rho_{II}$ are determined by requiring $\psi_1(x)$ and $\psi'_1(x)$ to be continuous at $x = \alpha$. In region I, when $x = \alpha+$, we have