Revised Iterative Solution for Groundstate of Schrödinger Equation* 

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(Received November 25, 2003)

Abstract A revised iterative method based on Green function defined by quadratures along a single trajectory is proposed to solve the low-lying quantum wave function for Schrödinger equation. Specially a new expression of the perturbed energy is obtained, which is much simpler than the traditional one. The method is applied to solve the unharmonic oscillator potential. The revised iteration procedure gives exactly the same result as those based on the single trajectory quadrature method. A comparison of the revised iteration method to the old one is made using the example of Stark effect. The obtained results are consistent to each other after making power expansion.

PACS numbers: 03.65.Ge, 02.30.Mv
Key words: single trajectory quadrature, Green function, revised iterative solution

1 Introduction

Recently a single trajectory quadrature method is proposed to solve the low-lying quantum states of N-dimensional Schrödinger equation.[1,2] The ground state wave function in N dimensions can be expressed by quadratures along the single trajectory. Furthermore a Green function is defined along the single trajectory.[2] This makes it possible to develop an iterative method for obtaining the ground state wave function, starting from a properly chosen trial function. The method is applied to solve one-dimensional double-well potential.[3] The convergence of the iterative solution very much depends on the choice of the trial function.

However, the solution based on this iterative formula is not completely the same as the one obtained from the single trajectory quadrature method. In the single trajectory quadrature method the wave function for the ground state is proposed to be in the form of an exponential, as it should be, while in the original iterative solution the obtained correction to the wave function is in the form of a power expansion. This sometimes leads to unreasonable results, as will be shown in the following.

In this work a revised version of the iterative solution is introduced, which is based on a different integral equation using the same set of Green functions. A new and much simpler expression of the energy correction is obtained. The solution is in an exponential form and the result is exactly the same as the one obtained based on the single trajectory method.

In Sec. 2, a brief introduction is given about the Green function method based on the single trajectory quadrature. Special discussion is given for the revision of the iterative formula. A comparison of the original and the revised version of the iterative solution is shown for a simple example. The revised iterative formula is then applied to the unharmonic oscillator potential and a comparison of the two iteration solutions is made using the example of the Stark effect in Sec. 3. Finally some discussions are given.

2 Green Function and Revised Iterative Solution

2.1 Green Function and Revised Iterative Formula

We discuss a particle with unit mass, moving in an N-dimensional unperturbed potential \( V_0(q) \). The ground state wave function \( \Phi(q) \) satisfies the following Schrödinger equation

\[
H\Phi(q) = E\Phi(q),
\]

where

\[
H = T + V_0(q) = -\frac{1}{2}\nabla^2 + V_0(q).
\]

Assume the solution of Eq. (1) could be expressed as

\[
\Phi(q) = e^{-S(q)},
\]

where \( S(q) \) is the trajectory based on which the Green function will be defined. From Eqs. (1) ~ (3) it is easy to derive the following equation for \( \hat{\mathcal{H}}(q) \)

\[
\frac{1}{2}(\nabla S)^2 - \frac{1}{2}\nabla^2 S - V_0 + E = 0.
\]

Introduce perturbed potential \( U(q) \) and assume

\[
V(q) = V_0(q) + U(q),
\]

\[
\hat{\mathcal{H}} = T + V(q) = -\frac{1}{2}\nabla^2 + V(q).
\]

Define another wave function \( \Psi(q) \) satisfying the Schrödinger equation,

\[
\hat{\mathcal{H}}\Psi(q) = E\Psi(q),
\]

\[
E = E + \Delta.
\]

Let

\[
\Psi(q) = e^{-S(q)-\tau(q)},
\]

The equation for \( \tau \) and \( \Delta \) could be derived easily,[2]

\[
\nabla S \cdot \nabla \tau + \frac{1}{2}[(\nabla \tau)^2 - \nabla^2 \tau] = (U - \Delta).
\]

Consider the coordinate transformation

\[
\theta_1, \theta_2, \ldots, \theta_N \rightarrow S, \theta_1, \alpha_2, \ldots, \alpha_N,
\]

with \( \alpha = (\alpha_1, \alpha_2, \ldots, \alpha_N) \) denoting the set of \( N-1 \) orthogonal angular coordinates satisfying the condition

\[
\nabla S \cdot \nabla \alpha_i = 0,
\]

for \( i = 1, 2, \ldots, N-1 \). Similar to the discussions in Ref. [2], introducing the \( \theta \)-function in \( S \)-space:

\[
\theta(S - \bar{S}) = \begin{cases} 
1, & \text{if } 0 \leq S < \bar{S}, \\
0, & \text{if } 0 \leq S < \bar{S},
\end{cases}
\]
and define
\[ C = \theta [(\nabla S)^2]^{-1}. \]

Using
\[ \nabla S \cdot \nabla C = 1, \]
it is easy to derive the following equation,
\[ \tau = \bar{G}[(U - \Delta) - \frac{1}{2}(\nabla \tau)^2] \]
\[ = (1 + CT)^{-1}C[(U - \Delta) - \frac{1}{2}(\nabla \tau)^2], \]
where the Green function \( \bar{G} = (1 + CT)^{-1}C \). From this equation and the expression of
\[ \Delta = \int \frac{\Phi^2(q) U e^{-\tau(q)} dq}{\int \Phi^2(q) e^{-\tau(q)} dq}, \]
the iteration process could be performed in the following way: Starting from \( \Delta_0 = 0 \) and \( \tau_0 = 0 \),
\[ \Delta_n = \int \frac{\Phi^2(q) U e^{-\tau_n - 1} dq}{\int \Phi^2(q) e^{-\tau_n - 1} dq}, \]
\[ \tau_n = (1 + CT)^{-1}C[(U - \Delta_n) - \frac{1}{2}(\nabla \tau_{n-1})^2]. \]
When the N-dimensional variable \( q \) is transformed into \( S, \alpha \), \( T = -\nabla^2/2 \) could be decomposed into two parts:
\[ T = T_S + T_\alpha, \]
where \( T_S \) and \( T_\alpha \) consist only the differentiation to \( S \) and \( \alpha \) respectively. The detailed expression of \( T_S \) and \( T_\alpha \) could be found in Appendix A.[2] Now another function could be defined as
\[ D \equiv -2\theta e^{2S} \int h_s^2 e^{-2S} h_s h_\alpha, \]
and it is related to the Green function \( \bar{G} \) and \( C \) in the following way:[2]
\[ \bar{G} = (1 + DT_\alpha)^{-1} \bar{D} = (1 + CT)^{-1}C. \]
Thus, the integral equation for \( \tau \) and \( \Delta \) could also be expressed as
\[ \tau = \bar{G}[(U - \Delta) - \frac{1}{2}(\nabla \tau)^2] \]
\[ = (1 + DT_\alpha)^{-1} \bar{D}[(U - \Delta) - \frac{1}{2}(\nabla \tau)^2] \]
\[ = \check{D}(1 + T_\alpha \bar{D})^{-1}[(U - \Delta) - \frac{1}{2}(\nabla \tau)^2]. \]
The explicit expression of \( \tau \) is
\[ \tau = -2\theta e^{2S} \int \frac{\Phi^2(q) U e^{-\tau(q)} dq}{\int \Phi^2(q) e^{-\tau(q)} dq} \times [(U - \Delta) - \frac{1}{2}(\nabla \tau)^2]. \]

Therefore, we have
\[ -\frac{1}{2} \int \frac{h_s e^{-2S} \partial \tau(S, \alpha)}{h_\alpha} dS \int \Phi^2(q) U e^{-\tau(q)} dq \times [(U - \Delta) - \frac{1}{2}(\nabla \tau)^2]. \]
The left-hand side of Eq. (25) approaches 0 when \( S \to \infty \), so is the right-hand side, i.e.,
\[ \int_0^\infty e^{-2S} h_s h_\alpha dS(1 + T_\alpha \bar{D})^{-1}[(U - \Delta) - \frac{1}{2}(\nabla \tau)^2] = 0, \]
which is correct for all \( \alpha \). Integrating over \( d\alpha \) gives
\[ \Pi_{n=1}^{N-1} d\alpha, \]
and of
\[ h_\alpha T_\alpha = -\frac{1}{2} \sum_{j=1}^{N-1} \frac{\partial h_s h_\alpha}{h_\alpha^2} \frac{\partial h_\alpha}{\partial \alpha_j}, \]
we derive
\[ \int h_s h_\alpha d\alpha dS e^{-2S} [(U - \Delta) - \frac{1}{2}(\nabla \tau)^2] = 0. \]
Denoting \( dq = h_s h_\alpha d\alpha dS \), we reach a new expression of the perturbative energy,
\[ \Delta = \int dq e^{-2S}[U - (\nabla \tau)^2/2] \]
\[ = \int dq \Phi^2[U - (\nabla \tau)^2/2]. \]

Based on Eqs. (23) and (30) we have another iteration series,
\[ \Delta_n = \int dq \Phi^2[U - (\nabla \tau_{n-1})^2/2], \]
\[ \tau_n = (1 + DT_\alpha)^{-1} \bar{D}[(U - \Delta_n) - \frac{1}{2}(\nabla \tau_{n-1})^2]. \]
Or, we can also use Eqs. (31) and (19), instead of Eqs. (18) and (19), as our iteration series, since the calculation of Eq. (31) is much simpler than Eq. (18).

Comparing the above iteration with the old one derived from the equations for \( f = e^{-\tau} \) and \( \Delta \),
\[ f_n = 1 + \bar{G}(-U + \Delta_n) f_{n-1}, \]
there are several advantages for the new one:

i) It directly gives an exponential form for the perturbed wave function \( e^{-\tau} \). This result is consistent with those obtained in the single trajectory quadrature method using the series expansion of \( \{S_i\} \) and \( \{E_i\} \) (See Sec. 1 of Ref. [2]).

ii) It makes the iteration more transparent, since there are no terms appearing as \( UF \) in the integration.

iii) The calculation of the perturbation energy is much simpler.

2.2 Example

This formula has been tried for several examples. In the following the result for a simple example will be given, with the one-dimensional potential
\[ V(x) = \frac{1}{2} g^2 x^2 + \lambda x. \]
Now we have
\[ V_0(x) = \frac{1}{2} g^2 x^2, \]
\[ U(x) = \lambda x, \]
and according to Eqs. (1) and (3),
\[ \Phi(x) = e^{-g x^2/2}, \]
\[ S(x) = \frac{1}{2} g x^2. \]
From Eqs. (14) and (15) we have, in this example,
\[ C = \theta \left( \frac{\partial S}{\partial x} \right)^{-2} = \int_0^x \frac{1}{g x} dx = \int_0^1 \frac{1}{g x} dx. \]
Define
\[ \Psi(x) = e^{-g x^2/2 - \tau(x)}. \]
Starting from \( \tau_0 = 0 \) and \( \Delta_0 = 0 \), based on Eqs. (18) and (19), we have
\[ \Delta_1 = \int_{-\infty}^\infty e^{-g x^2/2} \lambda x dx = 0. \]
The next step gives
\[ \Delta_2 = \int_{-\infty}^{\infty} e^{-\lambda x^2} dx \frac{\lambda^2}{2g^2} \]
Further iterations gives
\[ \tau_2 = (1 + CT)^{-1} C [U - \Delta_2] - \frac{1}{2} (\nabla \tau_1)^2 = \tau_1 . \]
The iteration is completed here and the obtained corrections for the ground state energy and wave function are
\[ \Delta = - \frac{\lambda^2}{2g^2} , \]
\[ \tau = \frac{\lambda}{g} x . \]
This is the exact solution of the ground state for the potential of Eq. (34).

In this section the revised iterative formula is applied on the Green functions defined in Eqs. (14), (21), and (22). And the result is compared to those obtained in Ref. [2] using the perturbation expansion based on the same set of Green functions.

**Example 1** Consider a one-dimensional harmonic oscillator with
\[ H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} g^2 x^2 , \]
and a perturbative potential
\[ U = \epsilon x^{2p} , \]
where \( p \) is a positive integer. The unperturbed ground-state wave function is
\[ \Phi = e^{-\delta} , \]
which satisfies Schrödinger equation,
\[ H\Phi(x) = E\Phi(x) . \]
Since \( S = gx^2/2 \), we have
\[ h_S^2 = \left( \frac{dS}{dx} \right)^{-2} = (gx)^{-2} = (2gS)^{-1} . \]
The eigenstate of
\[ H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} g^2 x^2 + \epsilon x^{2p} \]
is \( \Psi(x) = e^{-\delta} \), which satisfies Schrödinger equation,
\[ H\Psi(x) = (E + \Delta)\Psi(x) . \]
For one-dimensional case, equation (22) becomes
\[ G = D = (1 + CT)^{-1} C . \]

The revised iterative formula now consist of Eqs. (19) or (32) for \( \tau_n \) and Eq. (31) for \( \Delta_n \) as
\[ \Delta_n = \int_{-\infty}^{\infty} dx e^{-\lambda x^2} \left[ \epsilon x^{2p} - (\tau_n')^2 / 2 \right] \]
\[ \tau_n = (1 + CT)^{-1} C \left[ \epsilon x^{2p} - \Delta_n - \frac{1}{2} (\tau_n')^2 \right] \]
\[ = D[\epsilon x^{2p} - \Delta_n - \frac{1}{2} (\tau_n')^2] . \]
Taking
\[ \tau_0(x) = 0 , \quad \Delta_0 = 0 , \]
based on the formula given in Appendix B, it is easy to obtain
\[ \Delta_1 = \int_{-\infty}^{\infty} dx e^{-\lambda x^2} \left[ \epsilon x^{2p} - (\tau_1')^2 / 2 \right] \]
\[ \tau_1 = (1 + CT)^{-1} C[\epsilon x^{2p} - D[\epsilon x^{2p} - \epsilon\Gamma_1] \]
\[ = \epsilon \sum_{m=1}^{p} \Gamma_{mp} x^{2m} , \]
\[ \tau_1' = \epsilon \sum_{m=1}^{p} 2m\Gamma_{mp} x^{2m-1} . \]
For the second order, we have
\[ \Delta_2 = \int_{-\infty}^{\infty} dx e^{-\lambda x^2} \left[ \epsilon x^{2p} - (\tau_2')^2 / 2 \right] \]
\[ = \epsilon \Gamma_1 p - \frac{1}{2} \epsilon^2 \sum_{m=1}^{P} \Gamma_{mp} \Gamma_{np} x_{m+n-1} . \]
Specially, for \( p = 2 \),
\[
\Delta_2 = \epsilon \frac{3}{(2g)^2} - \epsilon^2 \frac{21}{8g^3}.
\]
The result is the same as those from the single trajectory quadrature method introduced earlier in Ref. [2]. When expanding \( e^{-r} \) to a power series, it is consistent to the perturbation expansion results obtained in Ref. [2] based on the same set of Green function.

**Example 2** Using the same one-dimensional harmonic oscillator Hamiltonian (51) as the unperturbed \( H \), we consider now an odd power perturbation potential, \( \epsilon U = \epsilon x^{2p+1} \).

With analysis parallel to that in the first example, using the formula introduced in Appendix B, starting from
\[
\tau_0(x) = 0, \quad \Delta_0 = 0,
\]
it is easy to obtain
\[
\Delta_1 = 0, \quad \tau_1 = (1 + CT)^{-1} C [\epsilon x^{2p+1}] = D [\epsilon x^{2p+1}]
\]
\[
= \frac{\epsilon}{2} \sum_{m=0}^{p} \gamma_{mp} x^{2m+1},
\]
\[
\tau_1' = \frac{\epsilon}{2} \sum_{m=0}^{p} (2m + 1) \gamma_{mp} x^{2m}.
\]

Similar to Eq. (64) we have, for \( p \neq 0 \),
\[
\Delta_2 = \int dx \, e^{-g x^2} |\epsilon x^{2p+1} - \{\tau_1\}^2/2|
\]
\[
- \frac{1}{2} \epsilon^2 \sum_{m=0}^{p} \sum_{n=0}^{p} (2m + 1)(2n + 1) \gamma_{mp} \gamma_{np} \Gamma_{1,m+n}.
\]

For the special case of \( p = 1 \), we have
\[
\Delta_1 = 0, \quad \tau_1 = \epsilon \left( \frac{1}{g^2} x + \frac{1}{3g} x^3 \right),
\]
\[
\Delta_2 = -\epsilon^2 \frac{11}{8g^2}, \quad \tau_2 = \tau_1 - \epsilon^2 \left( \frac{3}{8g^2} x^2 - \frac{1}{8g} x^4 \right).
\]
The result of \( p = 0 \) is already shown as the simple example at the end of Sec. 2. These results are exactly the same as those obtained based on the single trajectory quadrature method. After expanding \( e^{-r} \) to a power series the result is consistent to the one based on the perturbation expansion using the same set of Green function in Ref. [2].

It is worth while to mention that the formula based on the Green function \( D \) has another advantage for one-dimensional case. Since the expression of \( \tau_n \) is a double integration, \( \tau_n' \) could always be expressed as a single integration, i.e., no differentiation is needed. Compared to the single trajectory quadrature method introduced in Ref. [2], this revised iteration method could reach the same result, however, it has much less restriction to the potential. Because of the existence of many times of derivatives in the earlier method it requires the potential being continuous and very smooth for high order derivatives, while the revised iteration formula based on \( D \) is more flexible and could even be applied to discontinuous potentials.

### 3.2 Stark Effect

As a simple multi-dimensional example we now discuss the Stark effect, making detailed comparison of the two iteration procedures. Let \( H \) be the unperturbed Hamiltonian for a Coulomb potential:
\[
H = -\frac{1}{2} \nabla^2 - \frac{\epsilon^2}{r}
\]
with \( \nabla^2 \) denoting the three-dimensional Laplacian, \( r \) the radius. Considering the Stark effect as perturbation, the corresponding Hamiltonian is
\[
\mathcal{H} = H + \epsilon r \cos \theta,
\]
where \( \theta \) is the polar angle, i.e.,
\[
r^2 = x^2 + y^2 + z^2, \quad z = r \cos \theta.
\]
The ground-state of \( H \), \( \Phi(r) = e^{-S} = e^{-\nabla^2 r} \), satisfies
\[
H \Phi(r) = E \Phi(r) = -\frac{1}{2} \nabla^2 \Phi(r),
\]
and the ground-state wave function of \( \mathcal{H} \) satisfies
\[
\mathcal{H} \Psi(r) = (E + \Delta) \Psi(r).
\]

Introducing
\[
\Psi(r) = e^{-S(r)-T(r)},
\]
the perturbative energy \( \Delta \) and the function \( T(r) \) introduced for the wave function in Eq. (78) could be solved iteratively based on the revised iterative formula Eq. (19) or (32) for \( \tau_n \) and Eq. (31) for \( \Delta_n \). The corresponding functions \( C \) and \( D \) used in the Green function \( G \) are expressed as (see Appendix C)
\[
C = \frac{1}{g^2} \int_0^r dr,
\]
\[
D = -2 \int_0^r \frac{dr}{r^2} e^{2g^2 r} \int_r^\infty dr' r'^2 e^{-2g^2 r'}.
\]

Using the definitions of the corresponding quantities in the spherical coordinate given in Appendix C, we can perform the following two iterations. The revised one is
\[
\Delta_n = \int dr \, e^{-2g^2 r} \left[ \epsilon r \cos \theta - (\nabla \tau_n - 1)^2/2 \right],
\]
\[
\tau_n = (1 + CT)^{-1} C [\epsilon r \cos \theta - \Delta_n - \frac{1}{2} (\nabla \tau_n - 1)^2]
\]
\[
= (1 + DT_n)^{-1} D [\epsilon r \cos \theta - \Delta_n - \frac{1}{2} (\nabla \tau_n - 1)^2],
\]

starting from \( \Delta_0 = 0 \) and \( \tau_0(r) = 0 \); and the old one is
\[
\Delta_n = \int dr \, e^{-2g^2 r} \epsilon r \cos \theta f_{n-1}(r),
\]
\[
f_n = 1 + (1 + CT)^{-1} C [\Delta_n - \epsilon r \cos \theta] f_{n-1}
\]
\[
= 1 + (1 + DT_n)^{-1} D [\Delta_n - \epsilon r \cos \theta] f_{n-1},
\]

starting from \( \Delta_0 = 0 \) and \( f_0(r) = 1 \). From the revised iteration formulae (81) and (82) it is easy to obtain
\[
\Delta_1 = \int dr \, e^{-2g^2 r} [\epsilon r \cos \theta] = 0,
\]
\[
\tau_1 = \epsilon \left( \frac{1}{2g^2} r^2 + \frac{4}{(2g^2)^2} \right) \cos \theta.
\]

To calculate \( \Delta_2 \) and \( \tau_2 \) we need
\[
(\nabla \tau_1)^2 = \epsilon^2 \left[ \frac{16}{(2g^2)^2} + \frac{8}{(2g^2)^4} r + \frac{1}{(2g^2)^2} r^2 \right]
\]
\[
+ \frac{3}{(2g^2)^2} r^2 \cos^2 \theta,
\]
and the obtained results are
\[
\Delta_2 = \int dr \, e^{-2g^2 r} \left[ \epsilon r \cos \theta - (\nabla \tau_1)^2/2 \right],
\]
\[
\int dr \, e^{-2g^2 r}.
\]
Further iteration will give
\[ \Delta_4 = e^2 \frac{36}{(2g^2)^2} + e^4 \left( \frac{3555}{64g^2} + O(e^6) \right). \]  
(90)

The result is exactly the same as those based on the single trajectory quadrature method. The old iteration based on Eqs. (83) and (84) gives
\[ \Delta_4 = \int d\tau e^{-2g^2 r^2} \cos \vartheta = 0, \]  
(91)
\[ f_4(r) = 1 - e^{\left( \frac{1}{2g^2} r^2 + \frac{4}{(2g^2)^2} \right)} \cos \vartheta. \]  
(92)

Further iteration gives
\[ \Delta_2 = \frac{1}{2g^2} \int d\tau e^{-2g^2 r^2} f_2(r), \]  
(93)
\[ f_2(r) = 1 - e^{\left( \frac{1}{2g^2} r^2 + \frac{4}{(2g^2)^2} \right)} \cos \vartheta \]
\[ \times \left[ 1 + 3 \cos^2 \vartheta + 7 \left( \frac{2g^2}{(2g^2)^2} \right)^2 (1 + \cos^2 \vartheta) \right]. \]  
(94)

From the above analysis the advantages of this revised iteration method can be seen clearly. Because it directly gives an exponential form for the perturbed wave function \( e^{-\tau} \), it sometimes gives better convergence than the old formula, like the case of unharmonic oscillator shown at the end of Sec. 2. The exponential form of the perturbed wave function also ensures the result of this revised iteration procedure to be consistent with those obtained using the series expansion of \( \{S_i\} \) and \( \{E_i\} \) based on the single trajectory quadrature (See Sec. 1 of Ref. [2]). When we look at the formula Eq. (80) for the calculation of the perturbation energy, it is completely new and much simpler than the one in the old iteration procedure (see Eq. (17)).

The expression of the perturbation energy in the old iteration method is similar to the one in the usual perturbation method. In the new iteration formula Eq. (30) the denominator does not change in each order of iteration. The expression of the energy and the wave function in each order of iteration is proposed to solve the low-lying quantum wave function for Schrödinger equation. The method is applied to solve the unharmonic oscillator potential. A detailed comparison of the revised iteration method to the old one is made using the example of Stark effect.

\[ \text{Acknowledgment} \]

The author is grateful to Prof. T.D. Lee for his continuous and substantial instructions and advice.

\section*{Appendix A}

For the convenience of applying the coordinate system \( \{S, \alpha\} \) the definition introduced in Ref. [2] is given in the following. Based on the set of \( N-1 \) angular variables defined in Eq. (11)
\[ \alpha = (\alpha_1(q), \alpha_2(q), \ldots, \alpha_{N-1}(q)), \]  
(A1)
each point \( q \) in the \( N \)-dimensional space will now be designated by
\[ (S, \alpha_1, \alpha_2, \ldots, \alpha_{N-1}), \]  
(A2)
instead of \( (q_1, q_2, q_3, \ldots, q_N) \). The corresponding line element can be written as
\[ dq = \hat{S} h_S dS + \sum_{j=1}^{N-1} \hat{\alpha}_j h_{\alpha_j} d\alpha_j, \]  
(A3)
the gradient is given by
\[ \nabla = \hat{S} \frac{1}{h_S} \frac{\partial}{\partial S} + \sum_{j=1}^{N-1} \hat{\alpha}_j \frac{1}{h_{\alpha_j}} \frac{\partial}{\partial \alpha_j}, \]  
(A4)
\[ T = -\frac{1}{2} \nabla^2 \]  
(A5)
can be decomposed into two parts:
\[ T = T_S + T_\alpha \]  
(A6)
with
\[ T_S = -\frac{1}{2h_S h_{\alpha}} \frac{\partial}{\partial S} \left( h_{\alpha} \frac{\partial}{\partial S} \right), \]  
(A7)
\[ T_\alpha = -\frac{1}{2h_S h_{\alpha}} \sum_{j=1}^{N-1} \frac{\partial}{\partial \alpha_j} \left( h_{\alpha} h_{\alpha_j} \frac{\partial}{\partial \alpha_j} \right), \]  
(A8)
in which
\[ h_\alpha = \prod_{j=1}^{N-1} h_j. \]  
(A9)
and
\[ h_S^2 = [\nabla S]^2 ]^{-1}, \]
\[ h_1^2 = [\nabla \alpha_1]^2 ]^{-1}, \ldots, h_j^2 = [\nabla \alpha_j]^2 ]^{-1}, \ldots \]  \hfill (A10)

The volume element in the q-space is
\[ d^N q = h_S h_\alpha dS d\alpha \]  \hfill (A11)

with
\[ d\alpha = \prod_{j=1}^{N-1} d\alpha_j. \]  \hfill (A12)

**Appendix B**

In the calculation of $\Delta_n$ and $\tau_n$ in Sec. 3 the following expressions introduced in Ref. [2] are needed. With the definition of $C$ and $D$ introduced in Eqs. (39) and (47), for $n > 0$,
\[ C x^{2n} = \int_0^S g_x^{2n} x^{2n} = \frac{1}{g(2n)} x^{2n}, \]  \hfill (A13)
\[ D x^{2n} - \Gamma_1 n = (1 + CT)^{-1} C x^{2n} - \Gamma_1 n \]
\[ = \sum_{m=1}^{n} \Gamma_{m,n} x^{2m}, \]  \hfill (A14)

where
\[ \Gamma_{n,n} = \frac{1}{g^{2n}}, \Gamma_{n-1,n} = \frac{2n - 1}{g^{2(2n - 2)}}, \]
\[ \Gamma_{m,n} = \frac{(2n - 1)(2n - 3) \cdots (2m + 1)}{m(2g)^{m-n+1}} \]
for $1 \leq m \leq n - 1$, \hfill (A15)

and in particular
\[ \Gamma_{1,n} = \frac{(2n - 1)!!}{(2g)^n}. \]  \hfill (A16)

For $n \geq 0$,
\[ C x^{2n+1} = \int_0^S g_x^{2S} x^{2n+1} = \frac{1}{g(2n+1)} x^{2n+1}. \]  \hfill (A17)

It is straightforward to establish the following:
\[ D x^{2n+1} = (1 + CT)^{-1} C x^{2n+1} = \sum_{m=0}^{n} \gamma_{m,n} x^{2m+1}, \]  \hfill (A18)

where
\[ \gamma_{n,n} = \frac{1}{g(2n+1)}, \gamma_{n-1,n} = \frac{n}{g(2n - 1)}, \]
\[ \gamma_{m,n} = \frac{n(n-1) \cdots (m+1)}{g^{n-m+1}(2m+1)} \]
for $0 \leq m < n$, \hfill (A19)

and in particular $\gamma_{0,n} = n! / g^{n+1}$.

It is convenient to extend the definitions of $\gamma_{m,n}$ and $\Gamma_{m,n}$, by defining
\[ \gamma_{m,n} = \Gamma_{m,n} = 0 \quad \text{for} \quad m > n, \]  \hfill (A20)
and $\Gamma_{0,n} = 0$.

**Appendix C**

For the special case of spherical coordinate in three dimensions and for the Coulomb potential we have $S = g^2 r$. Correspondingly,
\[ \alpha = (\vartheta, \varphi), \quad h_S = 1, \quad h_\alpha = r, \quad h_\varphi = r \sin \vartheta. \]  \hfill (A21)

For any function $f(r)$ we have
\[ (\nabla f(r))^2 = \left( \frac{\partial f}{\partial r} \right)^2 + \left( \frac{1}{r \sin \vartheta} \frac{\partial f}{\partial \varphi} \right)^2, \]  \hfill (A22)
and $L^2$ is the operator of the square of the angular momentum. The Green functions used in the iteration are defined as
\[ G = (1 + DT_\alpha)^{-1} D = (1 + CT)^{-1} C. \]  \hfill (A23)

Assuming $\Psi(0) = \Phi(0)$ and $\Psi(r \rightarrow \infty) = 0$, we have
\[ C = \frac{1}{g^2} \int_0^r d r, \]  \hfill (A24)
\[ D = -2 \int_0^r d r \frac{1}{r^2} e^{2g^2 r} \int_r^\infty d r' r'^2 e^{-2g^2 r'}. \]  \hfill (A25)

In the iteration the following formula are applied,
\[ (1 + CT)^{-1} C r^n = \frac{1}{g^2} \sum_{m=2}^{n+1} \Lambda_{m,n} r^m + \Lambda_{1,n} (1 + CT)^{-1} C \cdot 1, \]  \hfill (A26)
\[ D r^n = \frac{1}{g^2} \sum_{m=2}^{n+1} \Lambda_{m,n} r^m + \Lambda_{1,n} D \cdot 1, \]  \hfill (A27)

where
\[ \Lambda_{n+1,n} = \frac{1}{n + 1}, \]
\[ \Lambda_{m,n} = \frac{1}{(2g^2)^{n+1-m} \frac{(n+2)(n+1) \cdots (m+2)}{m}}, \]
\[ \Lambda_{1,n} = -\frac{1}{(2g^2)^n} (n+2)(n+1) \cdots 3. \]  \hfill (A28)

Although $D \cdot 1 = (1 + CT)^{-1} C \cdot 1$ is divergent, all terms including this factor are cancelled in the iteration. Defining $\cos \vartheta = \xi$ we have $r^2 T_n \xi = \xi$ and
\[ r^2 T_n e^m = m \left( \frac{m+1}{2} e^m - \frac{m-1}{2} e^{m-2} \right). \]  \hfill (A29)

For Legendre function $P_l(\xi)$, we have
\[ r^2 T_n P_l(\xi) = \frac{l(l+1)}{2} P_l(\xi). \]  \hfill (A30)

Based on the above formula the two iteration procedures could be performed.

**References**

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