Iterative Solution for Generalized Sombrero-shaped Potential in $N$-dimensional Space

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Abstract

An explicit convergent iterative solution for the lowest energy state of the Schroedinger equation with generalized $N$-dimensional Sombrero-shaped potential is presented. The condition for the convergence of the iteration procedure and the dependence of the shape of the groundstate wave function on the parameters are discussed.

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1. Introduction

In this paper, the iterative method of Friedberg, Lee and Zhao[1] will be applied to a generalized radially symmetric Sombrero-shaped potential in \( N \)-dimensional space with

\[
V(r) = \frac{1}{2} g^2 (r^2 - r_0^2)^2 (r^2 + A r_0^2),
\]

where \( r_0^4 = (2 + N)/3 \), \( g^2 \) and \( A \) are arbitrary constants. The same potential in the special case of \( N = 1 \) has been studied recently[2]. As noted in Ref.[2] this investigation is stimulated by an interesting question raised by Roman Jackiw[3]. For arbitrary \( N \), the corresponding Schroedinger equation for the groundstate radial wave function is

\[
\left(-\frac{1}{2r^{2k}} \frac{d}{dr} r^{2k} \frac{d}{dr} + V(r)\right)\psi(r) = E\psi(r)
\]

with \( k = (N - 1)/2 \). The boundary conditions are

\[
\psi(\infty) = 0 \quad \text{and} \quad \psi'(0) = 0.
\]

When \( g = 1 \) and \( A = 2 \) the solution of the groundstate has an analytical form as \( \psi(r) = e^{-r^4/4} \) with the eigenvalue \( E_0 = r_0^6 \). However, for arbitrary \( g \) and \( A \) the groundstate wave function has no analytical form.

To apply the iterative method we introduce a trial function \( \phi(r) \) satisfying another Schroedinger equation

\[
\left(-\frac{1}{2r^{2k}} \frac{d}{dr} r^{2k} \frac{d}{dr} + V(r) - h(r)\right)\phi(r) = gE_0\phi(r) = (E - \Delta)\phi(r),
\]

where \( h(r) \) and \( \Delta \) are the corrections of the potential and the groundstate energy. The explicit construction of the trial function \( \phi(r) \) will be given in the next section. Here, we note some useful relations.

Multiplying (4) on the left by \( \psi(r) \) and (2) by \( \phi(r) \), their difference gives

\[
-\frac{1}{2r^{2k}} \frac{d}{dr} \left( \psi r^{2k} \frac{d}{dr} \phi - \phi r^{2k} \frac{d}{dr} \psi \right) = (h - \Delta)\phi\psi.
\]

Let

\[
\psi(r) = \phi(r) f(r).
\]
The equations for $f(r)$ and $\Delta$ can be deduced by using
\[
\frac{d}{dr} \left[ r^{2k} \phi^2 \frac{df}{dr} \right] = 2r^{2k}(h - \Delta)\phi^2 f. \tag{7}
\]

The integration of the left-hand side of (7) over $r = 0$ to $\infty$ is zero. This gives the expression of the energy correction
\[
\Delta = \frac{\int_0^\infty r^{2k} \phi^2(r) h(r) f(r) dr}{\int_0^\infty r^{2k} \phi^2(r) f(r) dr}. \tag{8}
\]

Introducing two iterative series $\{f_n(r)\}$ and $\{\Delta_n\}$ with $n = 0, 1, \cdots$, we obtain the following iteration equations
\[
\Delta_n = \frac{\int_0^\infty r^{2k} \phi^2(r) h(r) f_{n-1}(r) dr}{\int_0^\infty r^{2k} \phi^2(r) f_{n-1}(r) dr}, \tag{9}
\]
\[
f_n(r) = f_n(r_c) - 2 \int_{r_c}^r \frac{dy}{y^{2k} \phi^2(y)} \int_{r_c}^y x^{2k} \phi^2(x) (\Delta_n - h(x)) f_{n-1}(x) dx, \tag{10}
\]
where $r_c$ could be chosen as $r_c = 0$ or $r_c = \infty$. To ensure the convergency of the iterative method it is necessary to construct the trial function in such way that the perturbed potential $h(r)$ is always positive (or negative) and finite everywhere. Specially, $h(r) \to 0$ when $r \to \infty$. In the following we construct the trial function for the iteration procedure. As we shall see, in the cases that we have examined the iterations give rapidly convergent results.
2. Trial Functions

We first introduce a trial function

\[ \phi_+(r) = \left( \frac{r_0 + a}{r + a} \right)^k e^{-gS_0(r) - S_1(r)} \]  

(11)

satisfying the following Schrödinger equation

\[ \left(-\frac{1}{r^{2k}} \frac{d}{dr} r^{2k} \frac{d}{dr} + V(r) - h_+(r)\right)\phi_+(r) = gE_0\phi_+(r) \]  

(12)

and the boundary condition

\[ \phi_+(\infty) = 0. \]  

(13)

Substituting (11) into (12), we compare terms with the same power of \( g \). From \( g^2 \)-terms we obtain

\[ S_0'(r) = \sqrt{2v} = (r^2 - r_0^2)\sqrt{r^2 + Ar_0^2}. \]  

(14)

To ensure \( h_+(r) \) satisfying the convergence condition, \( S_1(r) \) is defined in a special way to prevent terms with positive powers of \( r \) presenting in \( h_+(r) \). For \( g^1 \) terms we have

\[ -\frac{1}{2} \left( 2S_0'S_1' - S_0'' - 2ka\sqrt{r^2 + Ar_0^2} \right)\bigg|_{r=r_0} - ka^2 = E_0. \]  

(15)

Introducing

\[ E_0 = E_0^{(1)} + E_0^{(2)} + E_0^{(3)} \]  

(16)

and defining

\[ E_0^{(3)} = -ka^2 \]  

(17)

we write

\[ S_0'S_1' = \left( \frac{1}{2}S_0'' - E_0^{(1)} \right) + (ka\sqrt{r^2 + Ar_0^2} - E_0^{(2)}). \]  

Since \( S_0'(r_0) = 0 \) we obtain

\[ E_0^{(1)} = \frac{1}{2}S_0''(r_0) = r_0^2\sqrt{1 + A}, \]  

(18)

\[ E_0^{(2)} = kar_0\sqrt{1 + A} \]  

(19)
and
\[ S'_1 = \left( \frac{1}{2} S''_0 - E_0^{(1)} \right) / S'_0 + \left( k a \sqrt{r^2 + A r_0^2} - E_0^{(2)} \right) / S'_0. \] (20)

Substituting \( S'_0(r) \) into (20) we have explicitly
\[ S'_1(r) = \frac{r(3 r^2 + 2 A r_0^2 - r_0^2) - 2 r_0^2 \sqrt{1 + A \sqrt{r^2 + A r_0^2}}}{2(r^2 - r_0^2)(r^2 + A r_0^2)} \]
\[ + \frac{k a}{\sqrt{r^2 + A r_0^2}(\sqrt{r^2 + A r_0^2} + r_0 \sqrt{1 + A})}. \] (21)

The expression for \( h_+(r) \) is
\[ h_+(r) = \frac{1}{2} \left( S'_1^2 - S''_1 \right) + \frac{1}{2} \frac{k(k + 1)}{(r + a)^2} - \frac{k a}{r(r + a)} S'_1 - \frac{k^2}{r(r + a)} \]
\[ + k a g(r_0^2 - a^2) \frac{\sqrt{r^2 + A r_0^2}}{r(r + a)} + k a^2 g \frac{A r_0^2}{r(\sqrt{r^2 + A r_0^2} + r)}. \] (22)

The condition \( \phi'(0) = 0 \) can be satisfied by introducing the trial function as
\[ \phi(r) = \phi_+(r) + \xi \phi_-(r) \quad \text{for} \quad r < r_0 \] (23a)
and
\[ \phi(r) = \left( 1 + \xi \phi_-(r_0) / \phi_+(r_0) \right) \phi_+(r) \quad \text{for} \quad r > r_0 \] (23b)

where \( \phi_-(r) \) is defined as
\[ \phi_-(r) = \left( r_0 + a \right) k \frac{e^{-g S_0(-r) - S_1(r)}}{r + a}. \] (24)

The parameter \( \xi \) is fixed to satisfy the condition \( \phi'(0) = 0 \), namely
\[ \phi'_+(0) + \xi \phi'_-(0) = 0. \] (25)

Correspondingly \( \phi(r) \) satisfies the Schroedinger equation (4) with
\[ h(r) = h_+(r) \quad \text{for} \quad r > r_0 \] (26)
and
\[ h(r) = h_+(r) + 2 g \xi \left( E_0 + k a \frac{a^2 - r_0^2}{r(r + a)} \sqrt{r^2 + A r_0^2} \right) \]
for \( r < r_0 \). It is interesting to notice that the condition (25) for \( \phi'(0) = 0 \) also ensures \( h(r) \) to be finite when \( r \to 0 \), which is necessary for the convergency of the iteration procedure.

By integrating (14) and (21) we obtain \( S_0(r) \) and \( S_1(r) \) as

\[
S_0(r) = \frac{1}{8} r \sqrt{r^2 + Ar_0^2} (2r^2 + Ar_0^2 - 4r_0^2) - \frac{1}{8} (A^2 r_0^4 + 4Ar_0^4) \ln(r + \sqrt{r^2 + Ar_0^2})
\]

\[
S_1(r) = \ln(r + r_0) + \frac{1}{4} \ln(r^2 + Ar_0^2) + \left( \frac{1}{2} + \frac{ka}{2r_0} \right) \ln \frac{\sqrt{1 + A\sqrt{r^2 + Ar_0^2}} + r + Ar_0}{\sqrt{1 + A\sqrt{r^2 + Ar_0^2}} - r + Ar_0}
\]

Substituting them into (12), (24) and (23a-b) gives the final expression of the trial function. From (21) we can also reach

\[
\frac{1}{2} (S_1'' - S_1') = \frac{\gamma}{8(r^2 + Ar_0^2)^2(\alpha + \beta)} + \frac{ka}{2r(r + a)(r^2 + Ar_0^2)} \frac{\gamma'}{\alpha' + \beta'}
\]

\[
+ \frac{k^2 a^2}{2(r^2 + Ar_0^2)(\sqrt{r^2 + Ar_0^2} + r_0\sqrt{1 + A})^2}
\]

\[
+ \frac{kar(2\sqrt{r^2 + Ar_0^2} + r_0\sqrt{1 + A})}{(r^2 + Ar_0^2)^{3/2}(\sqrt{r^2 + Ar_0^2} + r_0\sqrt{1 + A})^2}
\]

where

\[
\gamma = \frac{\alpha^2 - \beta^2}{(r^2 - r_0^2)^2}, \quad \gamma' = \frac{\alpha'^2 - \beta'^2}{(r^2 - r_0^2)^2}
\]

with

\[
\alpha = 15r^6 + (18A - 6)r^4r_0^2 + (8A^2 + 12A + 7)r^2r_0^4 + (8A^2 + 2A)r_0^6,
\]

\[
\beta = 8\sqrt{1 + Ar_0^2}r \left( 3r^2 + (2A - 1)r_0^2 \right) \sqrt{r^2 + Ar_0^2},
\]

\[
\alpha' = r(3r^2 + (2A - 1)r_0^2)
\]

and

\[
\beta' = 2r_0^2\sqrt{1 + Ar^2 + Ar_0^2}.
\]
Explicitly
\[
\gamma = 225r^8 + 270(1 + 2A)r^6r_0^2 + 3(188A^2 + 216A - 5)r^4r_0^4 \\
+36A(8A^2 + 10A - 1)r^2r_0^6 + 4(16A^4 + 8A^2 + 1)r_0^8
\]
and
\[
\gamma' = 9r^4 + 3(4A - 1)r^2r_0^2 + 4A(1 + A)r_0^4.
\]
Substituting (30) into (22) and (27) gives the final expression of \(h\). With above results for \(h\) and \(\phi\) we are ready to perform the iteration.

3. Numerical Result

Starting from the above defined trial function \(\phi(r)\) and the related \(h(r)\), we can perform the iteration based on (9) and (10). Our numerical results show that the finally obtained wave functions and eigenvalues for the groundstate convergent nicely. Let us take \(N = 3\) as an example.

For \(g = 1\) and \(A = 2\), the exact solution of the groundstate is
\[
\phi(x) = e^{-r^4/4}
\]
with \(E_0 = r_0^6\). Starting from the trial function defined by (23a) and (23b), with arbitrarily chosen parameter \(a\) and the corresponding parameter \(\xi\) fixed by (25), the iteration procedure (9) and (10) gives the final convergent result of the wave function and the eigenvalue of the groundstate, which is consistent to the exact solution. The trial function and the convergent groundstate wave function after the iteration are plotted in Fig. 1. It is interesting to observe the transition of the shape of the wave function for the trial function with maxima at a finite \(r\) to the final convergent one with only one maximum at \(r = 0\), as the exact groundstate wave function should be. This answered the question raised by R. Jackiw[3] in \(N\)-dimensional case: Even the trial function proposed has its maxima at \(r > 0\) the iteration procedure would still reach the exact solution of the groundstate wave function with its only maximum at \(r = 0\).

As examples the obtained groundstate wave functions after the iteration procedure are plotted in Figs. 2 and 3 for \(A = 2\) and \(g = 0.5, 1\) or \(2\), and for
$g = 1$ and $A = 1, 2$ or 3, respectively. In Table 1 the corresponding eigenvalues of the groundstate obtained from the iteration are listed for different parameters $g$ and $A$. It can be seen that the iterative energy series convergent quite nicely. From the figures it is interesting to see the transition of the form of the obtained groundstate wave functions from the shape with maximum at $r = 0$ to the one with maxima at a finite $r$, becoming a degenerate groundstate, when $g$ increases from $<1$, passing 1 to $>1$ for $A = 2$, or when $A$ increases from $<2$, passing 2 to $>2$ for $g = 1$. The results seem to show that the groundstate wave functions in the region $g \leq 1$ and $A \leq 2$ have the shape with only one maximum at $r = 0$, while in the region outside the wave functions become degenerate at a finite $r$. Their maxima move to larger $r$ when the parameters $g$ and $A$ increase further.

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| $g$ | $A$ | $gE_0$ | $gE_1$ | $gE_2$ | $gE_3$ | $gE_4$ | $gE_5$ |
|-----|-----|--------|--------|--------|--------|--------|--------|
| 0.5 | 2   | -0.4300| 1.3963 | 1.3795 | 1.3775 | 1.3773 | 1.3772 |
| 1   | 2   | -8.6479| 2.1523 | 2.1516 | 2.1517 | 2.1517 | 2.1517 |
| 2   | 2   | 5.5581 | 4.1362 | 4.0976 | 4.1108 | 4.1092 | 4.1094 |
| 1   | 1   | -2.3537| 1.8920 | 1.8473 | 1.8402 | 1.8393 | 1.8392 |
| 1   | 3   | 3.6773 | 2.4675 | 2.4353 | 2.4425 | 2.4417 | 2.4418 |
Fig. 1 Trial Function \( \phi(r) \) and Groundstate Wave Function \( \psi(r) \) for \( N = 3, \ g = 1 \) and \( A = 2 \).

Fig. 2 Groundstate Wave Function \( \psi(r) \) for \( N = 3, \ g = 1 \) and \( A = 1 \) (thin), 2 (middle) and 3 (thick).
Fig. 3 Groundstate Wave Function $\psi(r)$ for $N = 3$, $A = 2$ and $g = 0.5$ (thin), 1 (middle) and 2 (thick).