1/N expansion for a Mie-type potential

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The large-N expansion has been used for solving the Schrödinger equation for a Mie-type potential. The ground-state energy and the corresponding wave function are obtained analytically up to six terms.

I. INTRODUCTION

In recent years the large-N expansion has been used for solving the Schrödinger equation.¹⁻⁴ In solid-state physics such expansions are well known,^{5,6} similar expansions being developed for quantum field theory.⁷⁻⁹ This method provides a good approximation for obtaining the low-lying spectrum of quantum-mechanical systems, in contrast with the WKB method. Furthermore, the method has the following advantages: It does not depend on the separation of the Hamiltonian into two terms, one exactly solvable and the other relatively small, and the calculation can be done using a simple algebraic recursion method.

In the present work we apply the 1/N expansion to obtain the ground-state energy and the corresponding wave function for a system bound by a Mie-type potential. The analytical expressions are derived for the first six terms.

II. THE METHOD AND CALCULATIONS

We wish to solve the Schrödinger equation for a special case of the Mie potential 10

$$V(r) = D_0 \left[\frac{k}{m-k} \left(\frac{\sigma}{r} \right)^m - \frac{m}{m-k} \left(\frac{\sigma}{r} \right)^k \right] .$$
(1)

By taking m = 2k and k = 1, it reduces to

$$V(r) = \frac{A}{r^2} - \frac{B}{r} \quad , \tag{2}$$

where $A = D_0 \sigma^2$ and $B = 2D_0 \sigma$. We assume that the generalization of the potential to N dimensions, N being the number of spatial dimensions, may be written as

$$V_N(r) = N^2 V(r) / 9 \quad . \tag{3}$$

For simplicity, we write the Schrödinger equation in N dimensions for the l = 0 case (with $\hbar = 1$)

$$\left(-\frac{1}{2\mu}\nabla_N^2 + V_N(r)\right)\Psi = E\Psi \quad . \tag{4}$$

Considering only the radial part ψ of Ψ and redefining $\psi = r^{(1-N)/2}\Phi$, Eq. (4) takes the form

$$\left(-\frac{1}{2\mu}\frac{d^2}{dr^2} + N^2 V_{\text{tot}}(r)\right)\Phi = E\Phi \quad , \tag{5}$$

where

$$V_{\text{tot}}(r) = \frac{(1 - 1/N)(1 - 3/N)}{8\mu r^2} + V(r)/9 \quad . \tag{6}$$

In the large-N limit the ground-state energy is defined as the minimum of the effective potential

$$V_{\rm eff}(r) = \frac{1}{8\mu r^2} + V(r)/9 \quad , \tag{7}$$

namely, $V_0 = V_{\text{eff}}(r_0)$, and $E_{\text{ground}} = N^2 V_0$, where $V_0 = C^2/(2\mu r_0^2) - B/9r_0$ with $r_0 = 9C^2/\mu B$ being the position where the minimum occurs; here we define $C^2 = (9 + 8\mu A)/36$.

To calculate the higher-order corrections to the energy, we define

$$\epsilon = -2\mu r_0^2 E \quad , \tag{8}$$

$$r = r_0(1+x)$$
 , (9)

and transform Eq. (5) into a Riccati equation by means of

$$\Phi(x) = e^{f(x)} \quad , \tag{10}$$

to obtain

$$\frac{d^2 f(x)}{dx^2} + \left(\frac{df(x)}{dx}\right)^2 + N^2 u(x) = \epsilon \quad , \tag{11}$$

where

$$u(x) = -2\mu r_0^2 \left[\left(\frac{3-4N}{8\mu N^2} + \frac{C^2}{2\mu} \right) \frac{1}{r_0^2 (1+x)^2} - \frac{B}{9r_0 (1+x)} \right]$$
(12)

We now expand

$$\epsilon = \sum_{n=-2}^{\infty} \epsilon_n (1/N)^n \tag{13}$$

and

$$\frac{df(x)}{dx} = \sum_{n=-1}^{\infty} g_n(x) (1/N)^n \quad . \tag{14}$$

Substituting these expansions into Eq. (11) and combining the terms of the same order in (1/N), we obtain the recurrence relations for ϵ_n and g_n ,

$$g_{-1}^{2}(x) + \left(\frac{2\mu r_{0}B}{9(1+x)} - \frac{C^{2}}{(1+x)^{2}}\right) = \epsilon_{-2} , \qquad (15a)$$

$$g'_{-1}(x) + 2g_{-1}(x)g_0(x) + \frac{1}{(1+x)^2} = \epsilon_{-1}$$
, (15b)

$$g'_0(x) + 2g_{-1}(x)g_1(x) + g_0^2(x) - \frac{3}{4(1+x)^2} = \epsilon_0$$
, (15c)

and for $n \ge 1$,

$$g'_{n}(x) + \sum_{m=0}^{n} g_{m}(x)g_{n-m}(x) + 2g_{-1}(x)g_{n+1}(x) = \epsilon_{n} \quad , \quad (15d)$$

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where a prime denotes differentiation with respect to x.

Since $E = N^2 V_0$ to order N^2 , one obtains $\epsilon_{-2} = C^2$ and $g_{-1}(x) = -Cx/(1+x)$, where the sign is fixed requiring that $\Phi(x) \to 0$ as $x \to \infty$. Using the recurrence relations, Eq. (15), we obtain the first six terms of ϵ_n and $g_n(x)$ as

$$\epsilon_{-2} = C^2 \quad , \tag{16a}$$

$$\epsilon_{-1} = -C + 1 , \qquad (16b)$$

$$\epsilon_{0} = (-C^{2} - 6C + 4)/(4C^{2}) , \qquad (16c)$$

$$\varepsilon_1 = (8C^3 - 4C^2 - 15C + 8)/(8C^4) , \qquad (16d)$$

$$\epsilon_2 = (-3C^4 + 40C^3 - 12C^2 - 35C + 16)/(16C^6) , \qquad (16e)$$

$$\epsilon_3 = (-104C^5 - 72C^4 + 560C^3 - 128C^2 - 315C + 128)/(128C^8)$$
(16f)

and

$$g_{-1}(x) = -Cx/(1+x)$$
, (17a)

$$g_0(x) = (C-1)(x+2)/[2C(1+x)] , \qquad (17b)$$

$$g_1(x) = \left[(2C^2 + 4C - 3)x + (6C^2 + 4C - 4) \right] / \left[\frac{8C^3(1+x)}{3} \right] , \tag{17c}$$

$$g_2(x) = \left[\left(-6C^3 + 6C^2 + 8C - 5 \right) x + \left(-6C^3 + 10C^2 + 8C - 6 \right) \right] / \left[16C^5(1+x) \right] ,$$
(17d)

$$g_3(x) = \left[\left(-8C^4 - 96C^3 + 60C^2 + 64C - 35 \right) x + 4 \left(-6C^4 - 24C^3 + 21C^2 + 16C - 10 \right) \right] / \left[128C^7 (1+x) \right] ,$$
(17e)

$$g_4(x) = \left[\left(72C^3 - 40C^4 - 288C^3 + 140C^2 + 128C - 63\right)x + 2\left(36C^5 - 44C^4 - 144C^3 + 90C^2 + 64C - 35\right) \right] / \left[256C^9(1+x) \right]$$

III. CONCLUSIONS

We calculated the first six terms of the ground-state energy, Eq. (16), and the corresponding wave function, Eq. (17), for a quantum-mechanical system bound by a special case of the Mie potential. The present results for the potential parameters A = 0 and B = 1 in Eq. (2), which corresponds to the Coulomb potential, namely, the hydrogenatom potential, coincide with the previous calculations.^{3,4}

For this particular case the energy terms in the expansion, Eq. (13), take the form

$$\epsilon_n = \frac{n+3}{4}, \quad n \ge -2 \quad . \tag{18}$$

The expansion then converges to $\frac{81}{16}$. Hence the groundstate energy from Eq. (8) is obtained -0.5 a.u. exactly. This value is the exact nonrelativistic H-atom ground-state energy.

The path-integral solution of the same potential was obtained recently,¹¹ and the resultant energy expression is

$$E_n = -\frac{2m}{\hbar^2} \frac{B^2}{4n^2} \ . \tag{19}$$

For the H-atom case this energy expression also gives -0.5a.u. exactly. The present result reproduces exactly the path-integral solution and the nonrelativistic Schrödinger equation solution.

Following the same procedure and choosing an appropriate wave function, one can easily compute the energy and wave function for the excited states.

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(16c)

(17f)