Improved shifted $1/N$ expansion

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A correction to the $1/N$-expansion method in quantum mechanics is presented. It actually improves the convergence when compared to previous versions of this technique, including the $1/N$ shifted version. By properly modifying the definition of the shifted parameter, the results are clearly better in the first approximation and the method becomes reliable for a much wider class of spherically symmetric potentials.

I. INTRODUCTION

Currently the Schrödinger equation is an important subject of study because of the large number of problems of physics requiring its solution. As it is known, this equation has exact solutions only for a handful of potentials and for this reason a large variety of approximation schemes have been developed. One of the most recent proposals is the $1/N$ expansion[1] and its modification as the so-called shifted $1/N$ expansion.[2] The $1/N$-expansion method is a pseudoperturbative technique in the sense that it proposes a perturbation parameter that is not directly related to the coupling constant. This is a fundamental feature that allows one to attack problems that do not involve a small coupling constant or Hamiltonians without a solvable strong term. This means that, in principle, one can handle any kind of potential and find an approximate solution by making use of this approximation. However, the approximation has been used, in general, in connection with spherically symmetric potentials.[2-5] The method starts by writing the original Schrödinger equation in an N-dimensional space and then it is assumed that N is sufficiently large. In this way a new effective potential can be defined and the kinetic energy becomes negligible, resulting in a semiclassical approach. Then, one makes a suitable change of variable, to center the problem at the minimum of this effective potential, called r_0. In spherically symmetric Hamiltonians the natural choice is the use of $x=k^{1/2}(r-r_0)/r_0$ as the new variable, where $k=N+2l$ and $l(l+N-2)\hbar^2$ is the extrapolated $l(l+1)\hbar^2$ eigenvalue. If one expands the resulting equation in powers of x, an analytical structure similar to the one of the one-dimensional anharmonic oscillator is found. Once the problem is collapsed to its actual dimension $N=3$, it simply rests the task of relating the coefficients of both equations in order to read the energy spectrum. Because the solution of the anharmonic oscillator is known as richly perturbed as one wants, one just cuts the corresponding series at the desired order of approximation.

II. DISCUSSION OF THE IMPROVED METHOD

Recently, a correction to the technique just described that is based on the introduction of a new parameter a has been proposed,[2] that is, an appropriated shift of k. Once a is introduced, the expansion parameter is $1/\bar{k}$, where $\bar{k}=k-a$. To make this paper self-contained we include explicitly the most important formulas of the shifted $1/N$ expansion that are the starting point of our proposal of improvement.

The radial Schrödinger equation in an N-dimensional space

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{(k-1)(k-3)\hbar^2}{8mr^2}+V(r)\right]u(r)=Eu(r) \tag{1}$$

is written as

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2\bar{k}^2}{8mr^2}[1-(1-a)/\bar{k}][1-(3-a)/\bar{k}]+V(r)\right]u(r)=Eu(r)\ . \tag{2}$$

It is essential to properly define the potential in the large-$\bar{k}$ limit to get useful results. For this reason a constant Q is introduced with the purpose of rescaling the potential in $\bar{k}^2$, that is the order of magnitude of the centrifugal barrier. Then

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\bar{k}^2\left[\frac{\hbar^2}{8mr^2}[1-(1-a)/\bar{k}][1-(3-a)/\bar{k}]+\frac{V(r)}{Q}\right]\right]u(r)=Eu(r)\ . \tag{3}$$

In that limit one naturally finds the effective potential

$$V_{\rm eff}(r)=\frac{\hbar^2}{8mr^2}+\frac{V(r)}{Q}\ , \tag{4}$$

whose minimum r_0 is given in principle by

$$4mr_0^3V'(r_0)=\hbar^2Q\ . \tag{5}$$

Now we move the origin to r_0 by means of the definition

$$x\equiv\bar{k}^{1/2}(r-r_0)/r_0 \tag{6}$$

and consequently perform a series expansion in powers of x about $x=0$ to get

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{\bar{k}\hbar^2}{8m}\left[1+\frac{3x^2}{\bar{k}}-\frac{4x^3}{\bar{k}^{3/4}}+\frac{5x^4}{\bar{k}^2}-\frac{6x^5}{\bar{k}^{3/2}}+\frac{7x^6}{\bar{k}^2}-\cdots\right]-(2-a)\frac{\hbar^2}{4m}\left[1-\frac{2x}{\bar{k}^{1/2}}+\frac{3x^2}{\bar{k}}-\frac{4x^3}{\bar{k}^{3/2}}+\frac{5x^4}{\bar{k}^2}-\cdots\right]\right.$$
$$+(1-a)(3-a)\frac{\hbar^2}{8m\bar{k}}\left[1-\frac{2x}{\bar{k}^{1/2}}+\frac{3x^2}{\bar{k}^2}-\cdots\right]+\frac{r_0^2\bar{k}}{Q}\left[V(r_0)+V''(r_0)\frac{r_o^2x^2}{2\bar{k}}+V'''(r_0)\frac{r_0^3x^3}{6\bar{k}^{3/2}}+V''''(r_0)\frac{r_0^4x^4}{24\bar{k}^2}\right.$$
$$\left.\left.+V^{(v)}(r_0)\frac{r_0^5x^5}{120\bar{k}^{5/2}}+V^{(v1)}(r_0)\frac{r_0^6x^6}{720\bar{k}^3}+\cdots\right]\right]\phi(x)=\frac{Er_0^2}{\bar{k}}\phi(x)\ . \quad (7)$$

On the other hand, the Schrödinger equation for a one-dimensional anharmonic oscillator is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\tfrac{1}{2}m\omega^2x^2+\varepsilon_0+P(x)\right]\phi(x)=\lambda\phi(x)\ , \quad (8)$$

where $P(x)$ is the perturbation term. Here, we use

$$P(x)=g^{1/2}(\varepsilon_1x+\varepsilon_3x^3)+g(\varepsilon_2x^2+\varepsilon_4x^4)$$
$$+g^{3/2}(\delta_1x+\delta_3x^3+\delta_5x^5)$$
$$+g^2(\delta_2x^2+\delta_4x^4+\delta_6x^6) \quad (9)$$

in order to compare our results with those of Ref. 2.

Now, cutting the series (7) to the same order in x and $\bar{k}$ as Eq. (8), we compare term by term both equations to define all the anharmonic oscillator parameters in terms of $\bar{k}$, Q, r_0, and the potential derivatives.

The following identifications are straightforwardly obtained:

$$\omega=\left[\frac{3\hbar^2}{4m^2}+r_0^4\frac{V''(r_0)}{mQ}\right]^{1/2}=\frac{\hbar}{2m}\left[3+r_0\frac{V''(r_0)}{V'(r_0)}\right]^{1/2}, \quad (10)$$

$$g=1/\bar{k},\quad \lambda=Er_0^2/\bar{k}\ ,$$
$$\varepsilon_0=\frac{\hbar^2\bar{k}}{2m}-(2-a)\frac{\hbar^2}{4m}+(1-a)(3-a)\frac{\hbar^2}{8m\bar{k}}+\frac{r_0^2\bar{k}}{Q}V(r_0)\ ,$$
$$\varepsilon_1=\frac{\hbar^2}{2m}(2-a),\quad \varepsilon_2=-\frac{3\hbar^2}{4m}(2-a)\ ,$$
$$\varepsilon_3=-\frac{\hbar^2}{2m}+r_0^5\frac{V^{(3)}(r_0)}{6Q},\quad \varepsilon_4=\frac{5\hbar^2}{8m}+r_0^6\frac{V^{(4)}(r_0)}{24Q}\ ,$$
$$\delta_1=-\frac{\hbar^2}{4m}(1-a)(3-a),\quad \delta_2=\frac{3\hbar^2}{8m}(1-a)(3-a)\ ,$$
$$\delta_3=\frac{\hbar^2}{m}(2-a),\quad \delta_4=-\frac{5\hbar^2}{4m}(2-a)\ ,$$
$$\delta_5=-\frac{3}{4}\frac{\hbar^2}{m}+r_0^7\frac{V^{(5)}(r_0)}{120Q},\quad \delta_6=\frac{7\hbar^2}{8m}+r_0^8\frac{V^{(6)}(r_0)}{720Q}\ . \quad (11)$$

The use of the standard Rayleigh-Schrödinger perturbation theory yields to analytic expressions for the terms of anharmonic-oscillator energy series, as functions of its parameters. For any value of the radial quantum number n and for any value of l, one obtains

$$E=S_0+S_1+S_2+S_3+\cdots\ , \quad (12)$$

giving rise to the partial sums

$$E_p\equiv\sum_{i=0}^{p}S_i\ , \quad (13)$$

with

$$S_0=\frac{1}{g^2}\left[\frac{\hbar^2}{8mr_0^2}+\frac{V(r_0)}{Q}\right], \quad (14)$$

$$S_1=\frac{1}{gr_0^2}\left[(n+\tfrac{1}{2})\hbar\omega-(2-a)\frac{\hbar^2}{4m}\right], \quad (15)$$

$$S_2=\frac{1}{r_0^2}\left[\frac{\hbar^2}{8m}(1-a)(3-a)+[(1+2n)\tilde{\varepsilon}_2+3\tilde{\varepsilon}_4(1+2n+2n^2)]-\frac{1}{\hbar\omega}[\tilde{\varepsilon}_1^2+6(1+2n)\tilde{\varepsilon}_1\tilde{\varepsilon}_3+(11+30n+30n^2)\tilde{\varepsilon}_3^2]\right], \quad (16)$$

$$S_3=\frac{g}{r_0^2}\left\{[(1+2n)\tilde{\delta}_2+3(1+2n+2n^2)\tilde{\delta}_4+5(3+8n+6n^2+4n^3)\tilde{\delta}_6]\right.$$
$$-\frac{1}{\hbar\omega}[(1+2n)\varepsilon_2^2+12(1+2n+2n^2)\tilde{\varepsilon}_2\tilde{\varepsilon}_4+2(21+59n+51n^2+34n^3)\tilde{\varepsilon}_4^2+2\tilde{\varepsilon}_1\tilde{\delta}_1+6(1+2n)\tilde{\varepsilon}_1\tilde{\delta}_3$$
$$+30(1+2n+2n^2)\tilde{\varepsilon}_1\tilde{\delta}_5+6(1+2n)\tilde{\varepsilon}_3\tilde{\delta}_1+2(11+30n+30n^2)\tilde{\varepsilon}_3\tilde{\delta}_3+10(13+40n+42n^2+28n^3)\tilde{\varepsilon}_3\tilde{\delta}_5]$$
$$+\frac{1}{\hbar^2\omega^2}[4\tilde{\varepsilon}_1^2\tilde{\varepsilon}_2+36(1+2n)\tilde{\varepsilon}_1\tilde{\varepsilon}_2\tilde{\varepsilon}_3+8(11+30n+30n^2)\tilde{\varepsilon}_2\tilde{\varepsilon}_3^2$$
$$+24(1+2n)\tilde{\varepsilon}_1^2\tilde{\varepsilon}_4+8(31+78n+78n^2)\tilde{\varepsilon}_1\tilde{\varepsilon}_3\tilde{\varepsilon}_4+12(57+183n+225n^2+150n^3)\tilde{\varepsilon}_3^2\tilde{\varepsilon}_4]$$
$$-\frac{1}{\hbar^3\omega^3}[8\tilde{\varepsilon}_1^3\tilde{\varepsilon}_3+108(1+2n)\tilde{\varepsilon}_1^2\tilde{\varepsilon}_3^2+48(11+30n+30n^2)\tilde{\varepsilon}_1\tilde{\varepsilon}_3^3$$
$$\left.+30(31+109n+141n^2+94n^3)\tilde{\varepsilon}_3^4]\right\}, \quad (17)$$

where

$$\tilde{\varepsilon}_j \equiv \frac{\varepsilon j}{(2m\omega/\hbar)^{j/2}}, \quad \tilde{\delta}_j \equiv \frac{\delta_j}{(2m\omega/\hbar)^{j/2}}, \quad j=1,2,\ldots . \tag{18}$$

Now the shift parameter is fixed from the requirement that the term S_1 vanishes, then

$$a = 2-2(2n+1)m\omega/\hbar . \tag{19}$$

For $N=3$, the constant Q should be such as to make identical Eqs. (1) and (3) (and not for every value of N as in Ref. 2). This requirement results in a fundamental constraint relation

$$1+2l+(2n+1)\left[3+r_0\frac{V''(r_0)}{V'(r_0)}\right]^{1/2} = \left[\frac{4mr_0^3}{\hbar^2}V'(r_0)\right]^{1/2} \tag{20}$$

that determines explicitly the value of r_0. With this value of r_0, one must determine ω, a, and every identified parameter, afterwards one has to compute the energy eigenvalues of $V(r)$.

Excellent results have been obtained with this correction for many different potentials, especially in the Coulomb-like or power-law-like cases resulting in a faster convergence than in the standard $1/N$ method.

Nevertheless, we have found that there is a large class of potentials for which the method does not provide the bound-state energies as well as expected. We refer, in particular to those potentials which do not have their minima at the origin.

In this case, the range of solubility of Eq. (20) implies the loss of, practically, all the information about the shape of the function $V(r)$ to the left of its minimum.

It is well known that due to Taylor's theorem, the value of a given analytical function can be calculated at any point x, just by evaluating all its derivatives at any point x_0. This means that the derivatives contain information about the function not only at x_0 but concerning any point of the axis.

Taking into account the fact that the series that gives the energy crucially depends on the solution of Eq. (20) and on the successive derivatives of V, evaluated at this point, one should go further in the sum that approximates the energy, in order to recuperate this information.

Our proposal consists in a modification of the definition of r_0 with the aim of adding more information about the potential. In this way we go beyond the standard shifted method that was designed to give a finite sum to express Coulomb and harmonic-oscillator eigenvalues.

Hence, we will define $r_0^{(m)}$, as the point that makes some partial sum of corrections to the first term of the series to vanish, i.e.,

$$\sum_{i=1}^{m} S_i(r_0^{(m)}) \equiv 0 . \tag{21}$$

Now we put this value in the constraint equation to determine a

$$3+2l-a = \left[\frac{4mr_0^{(m)3}}{\hbar^2}V'(r_0^{(m)})\right]^{1/2} . \tag{20'}$$

The fact that $\sum_i S_i$ is a functional containing higher-order derivatives of $V(r)$, allows us to recuperate much of the features of $V(r)$ that were lost in the old definition of r_0.

III. EXAMPLES AND APPLICATIONS

In order to illustrate our proposal we present a comparison of the results given by the shifted method and those derived with our improved shifted one. We compute the energy levels of two potentials, one with its minimum at the origin and another displaced. For the first class we have chosen the Yukawa potential, in order to compare it with the results of Ref. 4. For the second group we have taken the Eckart potential.[6] This Eckart

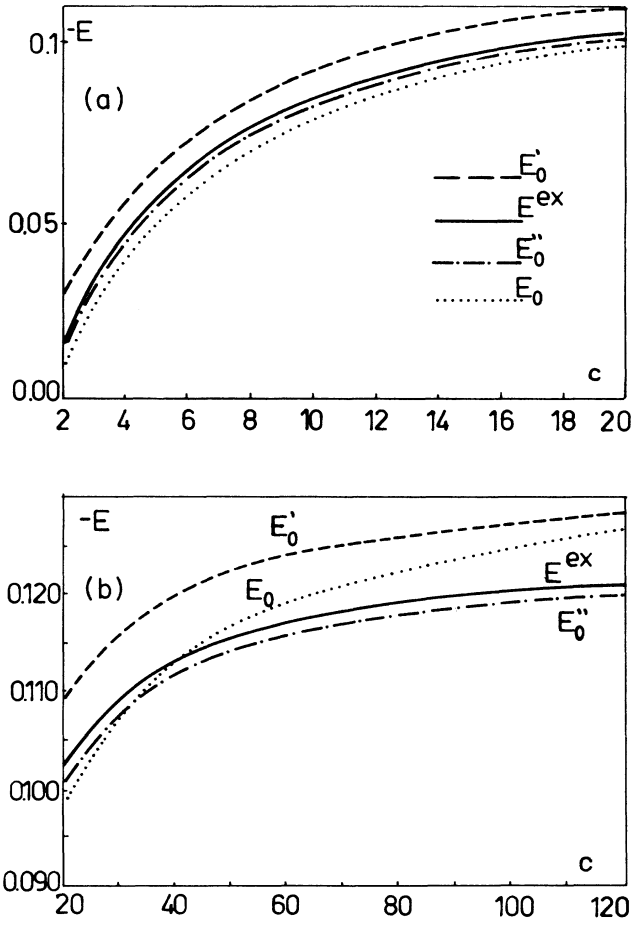

FIG. 1. Bound states ($n=l=0$) energy of the Eckhart potential as a function of the parameter c. The solid line corresponds to the exact solution (Ref. 6). E_0, E_0', and E_0'' are the leading terms of the shifted expansions corresponding to $S_1=0$, $S_1+S_2=0$, and $S_1+S_2+S_3=0$, respectively. The units are $\hbar=m=1$.

TABLE I. Energy eigenvalues versus δ for six Yukawa eigenstates. E_{num} is the numerically obtained energy from Ref. 7. The screening parameter is defined by (Ref. 4) $\delta = mA/b\hbar^2$ and $V(r) = Ae^{-br}/r$. E_0 is the standard shifted leading term, E_o' is the leading term when $S_1 + S_2 = 0$, and E_0'' corresponds to $S_1 + S_2 + S_3 = 0$. The energy units are $A^2 = 2\hbar^2/m$ (Ref. 4).

(n,l)	δ	$-E_0$	$-E_0'$	$-E_0''$	$-E_{\text{num}}$
(0.0)	500	0.996 00	0.996 00	0.996 00	0.996 0
	100	0.980 14	0.980 15	0.980 15	0.980 1
	10	0.814 22	0.814 11	0.814 11	0.814 1
	2	0.299 11	0.296 29	0.296 21	0.296 2
	1	0.003 28	0.148 87	0.015 30	0.020 57
(2.0)	200	0.101 51	0.101 44	0.101 44	0.101 4
	100	0.092 67	0.092 39	0.092 40	0.092 40
	70	0.085 64	0.085 11	0.085 12	0.085 12
	20	0.042 84	0.037 84	0.039 04	0.038 70
	10	0.012 70	−0.007 52	0.011 19	0.006 42
(1.1)	200	0.101 44	0.101 42	0.101 42	0.101 4
	100	0.092 40	0.092 31	0.092 31	0.092 31
	70	0.085 11	0.084 93	0.084 94	0.084 94
	20	0.038 55	0.036 92	0.037 16	0.037 12
	10	0.004 54	0.000 29	0.003 78	0.003 18
(4.2)	1000	0.018 48	0.018 48	0.018 48	0.018 48
	500	0.016 71	0.016 68	0.016 68	0.016 68
	200	0.012 16	0.011 97	0.011 98	0.011 98
	100	0.006 68	0.006 05	0.006 19	0.006 16
	70	0.003 53	0.002 36	0.003 01	0.002 83
(8.0)	1500	0.011 08	0.011 06	0.011 06	0.011 06
	1000	0.010 49	0.010 46	0.010 46	0.010 46
	500	0.008 91	0.008 79	0.008 79	0.008 79
	300	0.007 15	0.006 84	0.006 87	0.006 87
	100	0.002 15	0.012 87	0.001 82	0.001 17
(0.8)	1500	0.011 05	0.011 05	0.011 05	0.011 05
	700	0.009 65	0.009 66	0.009 66	0.009 66
	300	0.006 55	0.006 55	0.006 55	0.006 55
	200	0.004 26	0.004 26	0.004 26	0.004 26
	150	0.002 33	0.002 33	0.002 33	0.002 33

potential, frequently used in molecular physics, reads

$$V(r) = -cb^2 e^{-br}(1 + ce^{-br})^{-2}, \quad b > 0, \quad c > 1$$

and presents only one bound state for each value of b and c, given exactly by[6]

$$E = -\frac{b^2}{8}(c-1)^2/(c+1)^2 .$$

In this case, the convergence of the shifted results is not good for the first approximation, as shown in Fig. 1(b). Requiring $S_1 + S_2 = 0$ we find that E_0' improves the situation in the sense that the convergence is uniform. Imposing now $S_1 + S_2 + S_3 = 0$, we observe even a further improvement. In other words, with only the leading term E_0'' one gets the value corresponding to the third approximation of the standard shifted method.

A good example of the first group of potentials is the Yukawa one. We can see the same favorable behavior as before in Table I. Note that $S_1 + S_2 + S_3 = 0$ give excellent results in the first approximation even when δ is near δ_c. This is another important goal of our proposal.

IV. FINAL COMMENTS

We have found that through the present proposal, one can obtain all the desired precision with the first term of the $1/\bar{k}$ series, as soon as one finds the solution $r_0^{(m)}$ of $\sum_{i=1}^{m} S_i = 0$. Of course, these calculations may be long and tedious but straightforward in principle as before. We have shown that giving a new direction to the concept of the shift parameter in the shifted $1/N$ expansion, we can extend the use of the method to a larger class of potentials: those not having their minima at the origin.

Before concluding, it could be of interest to comment on the dependence of the results on the radial quantum number n that, in this respect, are entirely similar to the $S_1 = 0$ case. The coefficients in the series (12) for the energy eigenvalues are polynomials on n of increasing degree. This suggests a divergent behavior for the series. However, the parameter $r_0^{(m)}$ is also n dependent, and for that reason there are some potentials for which that series is in fact convergent, both in the standard shifted method[2] and in our present proposal. On the other hand,

whenever ω depends on r_0, the convergence is in question because in this case a is not a linear function of n. This is the case of potentials with an exponential screening (see, e.g., Refs. 4 and 5).

After the completion of this paper we became aware of Ref. 8, where similar ideas for improving the shifted $1/N$ expansion were presented, but in a more involved context. Moreover, our practical motivation was to solve, in a direct way, the problems present in the standard shifted $1/N$ expansion when treating potentials with their minima outside the origin of coordinates.

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