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## Shifted $1/N$ expansions for energy eigenvalues of the Schrödinger equation

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The $1/N$ expansion is a useful way of solving the Schrödinger equation to very high orders. We present a modified, physically motivated approach, called the shifted $1/N$ expansion, which dramatically improves the analytic simplicity and convergence of the perturbation series for the energy eigenvalues.

Recently it has been shown that the $1/N$ expansion is a powerful new way of solving the Schrödinger equation.[1-5] The techniques developed in $1/N$ expansions in nonrelativistic quantum mechanics have potential applications in quantum field theory where many interesting results have already been obtained in the large-$N$ limit.[6] A similar method is also well known in solid-state physics and is called the $1/S$ expansion, $S$ being the spin.[7] In nonrelativistic quantum mechanics, the method has mainly been applied to spherically symmetric potentials where the expansion parameter is $k=N+2l$, $N$ being the number of spatial dimensions and $l$ the eigenvalue of the $N$-dimensional orbital angular momentum.[4,5] For the case of power-law potentials $V(r)=Ar^{\nu}$, analytic expressions have been obtained to many orders in $1/k$. This is possible due to the advent of logarithmic perturbation theory,[1,8] which greatly simplifies calculations. These expressions, however, become progressively much more complicated, although providing good numerical results.[5] We present a somewhat modified novel approach which we shall call the shifted $1/N$ expansion. This method is physically motivated by the known exact analytic solutions of the power-law potential with $\nu=2$ (harmonic oscillator) and $\nu=-1$ (Coulomb potential). These results suggest that a desirable expansion parameter is $\bar{k}=k-a$, obtained by suitably shifting $k$. In this paper we demonstrate that this shift dramatically improves the simplicity of the analytic expressions and the convergence of the perturbation series for the energy eigenvalues. Our simple analytic forms give excellent agreement with numerical results. Throughout this article we will develop the shifted $1/N$ expansion for power-law potentials.

The radial Schrödinger equation in $N$ spatial dimensions is[4,5]

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{(k-1)(k-3)\hbar^2}{8mr^2}+Ar^{\nu}\right]\phi(r)=E\phi(r)\ , \tag{1}$$

where $k=N+2l$. The characteristic length and energy involved in this problem are

$$r_c\equiv\left[\frac{\hbar^2}{2mA}\right]^{1/(\nu+2)}\ ,\quad E_c\equiv Ar_c^{\nu}=\frac{\hbar^2}{2m}\left[\frac{2mA}{\hbar^2}\right]^{2/(\nu+2)}\ . \tag{2}$$

We scale out these characteristic quantities by defining the dimensionless variables

$$\xi=\frac{r}{r_c}\ ,\quad \lambda=\frac{E}{E_c}\ . \tag{3}$$

In order to get a useful $1/k$ expansion it is customary to define[4]

$$\eta=\xi k^{-2/(\nu+2)}\ . \tag{4}$$

We use a more general shifted variable $\bar{k}=k-a$ as an expansion parameter. For now $a$ is an additional degree of freedom. We shall motivate a convenient choice of $a$ later. The radial Schrödinger equation now reads

$$\left[-\frac{1}{\bar{k}^2}\frac{d^2}{d\eta^2}+\frac{\left(1-\frac{1-a}{\bar{k}}\right)\left(1-\frac{3-a}{\bar{k}}\right)}{4\eta^2}+\eta^{\nu}\right]\phi=\lambda\bar{k}^{-2\nu/(\nu+2)}\phi\ . \tag{5}$$

For large $\bar{k}$, the effective potential is $V_{\rm eff}=\eta^{\nu}+1/4\eta^2$ which has a minimum at $\eta_0=(1/2\nu)^{1/(\nu+2)}$. We now shift to this minimum by defining the variable $x=\bar{k}^{1/2}(\eta/\eta_0-1)$. Expanding about the point $x=0$ yields

$$\left[-\frac{d^2}{dx^2}+\frac{\bar{k}}{4}\left(1+\frac{3x^2}{\bar{k}}-\frac{4x^3}{\bar{k}^{3/2}}+\frac{5x^4}{\bar{k}^2}-\frac{6x^5}{\bar{k}^{5/2}}+\frac{7x^6}{\bar{k}^3}-\cdots\right)\right.$$
$$-\left(1-\frac{a}{2}\right)\left(1-\frac{2x}{\bar{k}^{1/2}}+\frac{3x^2}{\bar{k}}-\frac{4x^3}{\bar{k}^{3/2}}+\frac{5x^4}{\bar{k}^2}-\cdots\right)+\frac{(1-a)(3-a)}{4\bar{k}}\left(1-\frac{2x}{\bar{k}^{1/2}}+\frac{3x^2}{\bar{k}}-\cdots\right)$$
$$\left.+\frac{\bar{k}}{2}\left(\frac{1}{\nu}+\frac{(\nu-1)x^2}{2!\bar{k}}+\frac{(\nu-1)(\nu-2)x^3}{3!\bar{k}^{3/2}}+\frac{(\nu-1)(\nu-2)(\nu-3)x^4}{4!\bar{k}^2}+\cdots\right)\right]\phi=\lambda\eta_0^2\bar{k}^{(2-\nu)/(\nu+2)}\phi\ . \tag{6}$$

 

The unperturbed problem is the harmonic oscillator with frequency $\omega=\sqrt{\nu+2}$; we treat all other terms as a perturbation. For $a=0$ it has been shown that[3,4]

$$E=E_c\lambda=k^{(\nu-2)/(\nu+2)}\left[\frac{4\nu Am}{\hbar^2}\right]^{2/(\nu+2)}\frac{\hbar^2}{m}\left[k\left(\frac{1}{8}+\frac{1}{4\nu}\right)+[\tfrac{1}{2}(n+\tfrac{1}{2})\sqrt{\nu+2}-\tfrac{1}{2}]\right.$$
$$+\frac{1}{k}\left(\frac{-2}{\nu+2}-\frac{3(n+\frac{1}{2})}{\sqrt{\nu+2}}-\tfrac{15}{144}(\nu-5)^2(n^2+n+\tfrac{11}{30})-\frac{(\nu-5)}{\sqrt{\nu+2}}(n+\tfrac{1}{2})\right.$$
$$\left.\left.+\tfrac{1}{16}(\nu^2-8\nu+27)(n^2+n+\tfrac{1}{2})+\tfrac{3}{8}\right)+O\left(\frac{1}{k^2}\right)\right] , \tag{7}$$

where $n=0,1,2,\ldots$ is the principal quantum number. Note that the analytic behavior of the energy in terms of the coupling constant is completely displayed in the factor $A^{2/(\nu+2)}$ which has to appear to make the dimensions that of energy.

For the case $\nu=2$ and $A=m\omega^2/2$, the exact analytic solution is known to be

$$E=\frac{\hbar\omega}{2}(k+4n) . \tag{8}$$

Indeed, only the first two partial sums in Eq. (7) survive in this case and Eq. (8) is reproduced. For $\nu=-1$ and $A=-e^2$, the complete analytic solution is also known and has the form

$$E=\frac{-2me^4}{\hbar^2(k+2n-1)^2} . \tag{9}$$

In this case Eq. (7) is, in fact, an infinite series. Clearly, it would be desirable to have an expansion that reproduces known exact analytic results immediately. This can be easily done by noting that Eqs. (8) and (9) involve a shifted $k$. The shift is such as to give an exact result after just one partial sum in the shifted variable. This motivates the use of an expansion parameter

$$\bar{k}=k-a , \quad a=2-(2n+1)\sqrt{\nu+2} , \tag{10}$$

where $a$ has been chosen so that when Eq. (10) is substituted into Eq. (7), the resulting $1/\bar{k}$ expansion will have the coefficient of $\bar{k}^0$ (inside the large square brackets) equal to zero. The result is

$$E=\bar{k}^{(\nu-2)/(\nu+2)}\left[\frac{4\nu Am}{\hbar^2}\right]^{2/(\nu+2)}\frac{\hbar^2}{m}\left\{\frac{\bar{k}(\nu+2)}{8\nu}-\frac{(\nu+1)(\nu-2)}{12^2\bar{k}}\left[(1+6n+6n^2)+O\left(\frac{1}{\bar{k}}\right)\right]\right\} . \tag{11}$$

For $\nu=-1,2$, Eqs. (8) and (9) are reproduced. Note that our result is much simpler than Eq. (7).

When $n=0$ it is possible to carry out the calculation to higher orders. This is most conveniently done with use of the logarithmic perturbation theory.[1,8] This has recently been done for $1/k$ expansions and yields explicit but very cumbersome algebraic expressions which are too long to write here [see Table IV (c) in Ref. 5]. We have solved Eq. (6) for $n=0$ which corresponds to

$$\bar{k}=k-(2-\sqrt{\nu+2}) . \tag{12}$$

The calculations using logarithmic perturbation theory are long but straightforward; they involve integrals over the unperturbed harmonic-oscillator ground-state wave function and the perturbing potential.[8] In particular, the method is simple since one does not need to sum over intermediate unperturbed eigenstates as in the standard Rayleigh-Schrödinger approach. Our result is

$$E=\bar{k}^{(\nu-2)/(\nu+2)}\left[\frac{4\nu Am}{\hbar^2}\right]^{2/(\nu+2)}\frac{\hbar^2}{m}\left\{\frac{\bar{k}(\nu+2)}{8\nu}-\frac{(\nu+1)(\nu-2)}{12^2\bar{k}}\right.$$
$$\left.\times\left[1-\frac{(\nu+1)(\nu-2)}{12\bar{k}\sqrt{\nu+2}}+\frac{(317\nu^4-166\nu^3-1923\nu^2-15\,364\nu-17\,164)}{225(12\bar{k}\sqrt{\nu+2})^2}+O\left(\frac{1}{\bar{k}^3}\right)\right]\right\} . \tag{13}$$

This is dramatically simpler than the $1/k$ result.[5] Note that in every partial sum after the first, $(\nu-2)$ $(\nu+1)$ appears as a factor. This assures us the exact answer again for $\nu=-1,2$ after one term. (Note that for $\nu=0$, $E=A$ as it should be.) Every subsequent term in the series will contain two more powers of $\nu$ in the numerator and an added factor of $\sqrt{\nu+2}$ in the denominator. Although the first few partial sums in the eigenvalue expansion are suggestive of an exact analytic form for the entire series, the $1/\bar{k}^3$ term breaks the pattern. Bringing the calculation to even higher

TABLE I. Comparison of the shifted $1/N$ expansion results with numerical ($N=3$) results (Ref. 9) (in parentheses) for various potentials ($\hbar=m=1$). The $n=0$ results were computed using the four partial sums displayed in Eq. (13); the excited states were computed using the two partial sums in Eq. (11).

| | | $V(r)$ | | |
|---|---|---|---|---|
| $l$ | $n$ | $-2^{1.7}r^{-0.2}$ | $-2^{0.8}r^{-0.8}$ | $2^{7/2}r$ |
| $l=0$ | 0 | −2.686 01 | −1.218 70 | 9.352 43 |
| | | (−2.686) | (−1.218) | (9.352 43) |
| | 1 | −2.258 63 | −0.464 61 | 16.266 79 |
| | | (−2.253) | (−0.462) | (16.351 8) |
| | 2 | −2.051 34 | −0.266 95 | 21.917 85 |
| | | (−2.044) | (−0.265) | (22.082 24) |
| $l=1$ | 0 | −2.344 94 | −0.500 44 | $V(r)=r^4$ |
| | | (−2.345) | (−0.500) | |
| | 1 | −2.102 32 | −0.281 05 | $n=l=0$ |
| | | (−2.101) | (−0.281) | |
| | 2 | −1.953 74 | −0.187 91 | 2.394 73 |
| | | (−1.951) | (−0.187) | (2.393 64) |
| $l=2$ | 0 | −2.156 26 | −0.294 70 | |
| | | (−2.156) | (−0.295) | |
| | 1 | −1.990 73 | −0.195 03 | |
| | | (−1.990) | (−0.195) | |
| | 2 | −1.876 59 | −0.142 21 | |
| | | (−1.875) | (−0.142) | |
| $l=3$ | 0 | −2.029 06 | −0.201 91 | |
| | | (−2.029) | (−0.202) | |
| | 1 | −1.905 21 | −0.146 39 | |
| | | (−1.905) | (−0.146) | |
| | 2 | −1.813 40 | −0.112 89 | |
| | | (−1.812) | (−0.113) | |

orders would be extremely difficult by hand. There do exist, however, various computer languages which perform algebraic manipulations that can proceed more efficiently. We also mention here that our expansion parameter $\bar{k}$, Eq. (10), is larger than the standard parameter $k$ for $\nu>2$, so that for these values we expect a more rapidly convergent series than a $1/k$ expansion. For $-2<\nu<2$, $\bar{k}$ is slightly less than $k$; however, having complete answers for $\nu=-1, 0, 2$ after one partial sum keeps the $1/\bar{k}$ series close to the exact answer in this region also.

Table I compares results from Eq. (11) for general $n$ and Eq. (13) for $n=0$ with numerical results[9] for various potentials. The accuracy of our results using $\bar{k}$ is much better than the $1/k$ expansion results obtained previously,[5] if one keeps terms to any given order. In a sense, the shifted parameter $\bar{k}$ has provided a physically motivated resummation of the perturbation series which improves its convergence. This is clearly a better approach than using a mathematical resummation technique such as Padé or a Shanks approximation. However, if desired, we can now further improve the convergence of our series in $1/\bar{k}$ by performing such a mathematical transformation.

To our knowledge, our main results [Eqs. (11) and (13)] are the simplest known analytic expressions for the energy eigenvalues of power-law potentials. It is clear that the $1/\bar{k}$ expansion method can be generalized to any spherically symmetric potential $V(r)$. As discussed before, the choice of the shift $a$ in $\bar{k}=k-a$ should be such as to make the second partial sum in the $1/k$ expansion vanish, thereby improving the rate of convergence of the energy eigenvalue perturbation series.

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