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Renormalization-group resummation of a divergent series of the perturbative wave functions of the quantum anharmonic oscillator

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The renormalization group method is applied to obtain the asymptotic form of the wave function of the quantum anharmonic oscillator by resumming the perturbation series. It is shown that the resummed series is the *cumulant* of the naive perturbation series. Working out up to the sixth order and performing the further resummation proposed by Bender and Bettencourt, we find that the agreement with the WKB result becomes worse in higher orders than the fourth, at which the agreement is the best. [S0556-2821(98)50104-X]

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It is well known that naive perturbation series are divergent or at best asymptotic series [1]. One needs to resum the divergent series to obtain a sensible result from perturbation theory. Indeed, various resummation techniques have been devised [1]. Recently, a unified and mechanical method for global and asymptotic analysis has been proposed by Goldenfeld *et al.* [2]. This is called the renormalization group (RG) method. The unique feature of their method is to start with naive perturbation theory and allow secular terms to appear in contrast with all previous methods [1]; adding unperturbed solutions to the perturbed solutions so that the secular terms vanish at a ''renormalization point'' $t=t_0$ and then applying the RG equation, one obtains a resummed perturbation series.

Subsequently, the present author formulated the RG method geometrically on the basis of the classical theory of envelopes [3]; it was indicated that the RG equation in the manner of Gell-Mann and Low in field theory can be identified as the envelope equation.

The purpose of the present work is to apply the RG method as formulated in [3] to the Schrödinger equation of the quantum anharmonic oscillator (AHO) and obtain the asymptotic form of the wave function.

The AHO is a theoretical laboratory for examining the validity of various approximation techniques [4,5]. Recently, Bender and Bettencourt [6] have shown that multiple-scale perturbation theory (MSPT) can be successfully applied to the quantum anharmonic oscillator; MSPT or the reductive perturbation theory is known to be one of the most general methods in applied mathematics [1] apart from the RG method for improving perturbative expansions [7]. They examined the Heisenberg operator equation and the (time-independent) Schrödinger equation: The exact closed-form solution was found for the Heisenberg equation, and the asymptotic behavior of the wave function $\psi(x)$ for large x was constructed, which agrees with the WKB result. One should remark here that a further resummation had to be adopted for the latter case, which is not intrinsic in MSPT and a similar method had been proposed by Ginsburg and Montroll [8].

Actually the RG method in the manner of Goldenfeld *et al.* has been already applied to quantum mechanics by others [9,10]: Egusquiza and Valle Basagoiti [9] applied it to solve the time-dependent Heisenberg equation considered in [6], while Frasca used it to solve the time-dependent Schrödinger equation of a two-level system. There has been, however, no attempt to apply the RG method to obtain asymptotic forms of wave functions. The reason may be that it is not trivial to identify the secular terms for the wave functions which can be made to vanish at a ''renormalization point'' $x=x_0$. In the present work, such secular terms are successfully identified for the ground and the first excited states.

We shall show that the resummation of the perturbation series of the wave functions is performed in the RG method more mechanically and explicitly than in MSPT: The polynomials $f_n(x)$ in the resummed series are explicitly given in terms of the polynomials $P_n(x)$ obtained in the naive perturbation theory [6]. Furthermore, it will be found that $\Sigma_{n=0}^{\infty}\epsilon^n f_n(x)$ is the *cumulant* series [11] of the naive perturbation series $\Sigma_{n=0}^{\infty}\epsilon^n P_n(x)$. Since our method is mechanical and easy to perform, we shall work out up to the sixth order in the perturbative expansion and examine how the results of Bender and Bettencourt persist or are modified in the higher orders.

Our Hamiltonian for the anharmonic oscillator is given by [12]

$$H=p^2+\tfrac{1}{4}x^2+\tfrac{1}{4}\epsilon x^4, \tag{1}$$

and we consider the following Schrödinger equation

$$(H-E)\psi(x)=0, \tag{2}$$

with the boundary condition $\psi(\pm\infty)=0$. We shall confine ourselves to the ground state for the moment. WKB analysis shows that for large x,

$$\psi(x)\sim\exp\{-\sqrt{\epsilon}|x|^3/6\}. \tag{3}$$

We shall examine how the perturbation theory can reproduce the WKB behavior or not, as was done in [6].

As preliminaries, we first apply the Bender-Wu method [14] for performing Rayleigh-Schrödinger (RS) perturbative expansion. The wave function and the eigenvalue are both expanded as power series of ϵ:

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$$\psi(x)\sim\sum_{n=0}^{\infty}\epsilon^n y_n(x) \quad \text{and} \quad E(\epsilon)\sim\sum_{n=0}^{\infty}\epsilon^n E_n. \tag{4}$$

We take the boundary values, hence the normalization as

$$y_0(0)=1 \quad \text{and} \quad y_{n\geqslant 1}(0)=0. \tag{5}$$

The lowest-order solution reads

$$y_0(x)=e^{-x^2/4} \quad \text{and} \quad E_0=1/2. \tag{6}$$

The higher-order terms with $n\geqslant 1$ are written as

$$y_n(x)=e^{-x^2/4}P_n(x), \tag{7}$$

where $P_n(x)$ is a polynomial. It is readily shown that the polynomials satisfy the recursion relation:

$$P_n''(x)-xP_n'(x)=\frac{x^4}{4}P_{n-1}(x)-\sum_{j=0}^{n-1}P_j(x)E_{n-j}. \tag{8}$$

This equation determines the polynomials and the eigenvalues E_n successively. Here it should be remarked that $y_n(x)$ in Eq. (7) may be identified as a secular term because it is a product of the unperturbed solution and a function that increases as x goes large.

The eigenvalues E_n are given by the condition (solvability condition) $\int_{-\infty}^{\infty}dxy_0(x)\hat{h}F(x)=0$, where $\hat{h}=(d/dx)^2-xd/dx$ and $F(x)$ is an arbitrary function with which the integral converges. Thus one finds

$$E_n=\frac{1}{2\sqrt{\pi}}\int_{-\infty}^{\infty}dxy_0(x)\left[\frac{x^4}{4}P_{n-1}(x)-\sum_{j=1}^{n-1}P_j(x)E_{n-j}\right]. \tag{9}$$

Note that E_n is determined in terms of only the polynomials $P_j(x)$ with $j\leqslant n-1$.

With these eigenvalues E_j $(j\leqslant n)$, the polynomial $P_n(x)$ is determined by Eq. (8). The general form of the polynomial is expressed as [6]

$$P_n(x)=\sum_{k=1}^{2n}C_{n,k}\left(-\frac{x^2}{2}\right)^k, \tag{10}$$

where the coefficient $C_{n,k}$ satisfies a recursion relation

$$2kC_{n,k}+C_{n-1,k-2}=-(k+1)(2k+1)C_{n,k+1}+\sum_{j=1}^{n-1}C_{j,k}C_{n-j,1}, \tag{11}$$

with $C_{n,1}=E_n$. The recursion relation is solved for low k with given n. The polynomials $P_n(x)$ up to the six order are presented in [6], which we refer to.

Now we apply the renormalization group method to resum the perturbation series obtained above. We shall present the method so that it becomes clear that the notion of envelopes is intrinsically related to the method [3]: We shall also make it clear that the RG method concerns with the boundary conditions in conformity with the general property of the RG methods as emphasized by Shirkov [13].

First we try to obtain the wave function $\psi(x;x_0)$ around an initial point $x=x_0$ in a perturbative way,

$$\psi(x;x_0)\sim\sum_{n=0}^{\infty}\epsilon^n z_n(x;x_0) \quad \text{and} \quad E(\epsilon)\sim\sum_{n=0}^{\infty}\epsilon^n E_n, \tag{12}$$

with the initial or boundary condition (BC) at $x=x_0$:

$$\psi(x_0;x_0)=W(x_0). \tag{13}$$

We suppose that the boundary value $W(x_0)$ is always on an exact solution of Eq. (2). $W(x_0)$ may be also expanded in a power series of ϵ:

$$W(x_0)=\sum_{n=0}^{\infty}\epsilon^n W_n(x_0). \tag{14}$$

If we stop at, say, the Nth order, we will have $\Sigma_{n=0}^{N}\epsilon^n z_n(x)\equiv\psi^{(N)}(x;x_0)$ which is valid only locally at $x\sim x_0$. However, one may take another point of view as follows: Geometrically, we have a family of curves $\{\psi^{(N)}(x;x_0)\}_{x_0}$ parametrized with x_0, and each curve of the family is a good approximation around $x=x_0$. Then, if each curve is continued smoothly, the resultant curve will be valid in a global domain of x. This is nothing else than to construct the envelope of the family of curves. More specifically, we only have to determine the boundary values $W_n(x_0)$ so that the perturbative solutions around $x=x_0$ form an envelope. This is the basic strategy of the RG method described geometrically. Furthermore, to be as accurate as possible, the lowest value $W_0(x_0)$ should approximate the exact value $\psi(x_0,x_0)$ as close as possible, or $W_{n\geqslant 1}(x_0)$ should be made as small as possible.

Let us perform the above program. First, we note that the lowest-order solution may be written as

$$z_0(x;x_0)=A(x_0)e^{-x^2/4}, \tag{15}$$

and $E_0=1/2$; we have made it explicit that the amplitude $A(x_0)$ may be dependent on x_0. The choice of the lowest-order solution implies that we have also chosen the boundary value as

$$W_0(x_0)=A(x_0)e^{-x_0^2/4}. \tag{16}$$

The higher-order terms with $n\geqslant 1$ may be written as

$$z_n(x;x_0)=A(x_0)e^{-x^2/4}Q_n(x;x_0), \tag{17}$$

where $Q_n(x;x_0)$ is a polynomial of x, dependent on x_0. It is readily shown that the polynomials satisfy the same recursion relation Eq. (8) as $P_n(x)$. However, since we want to make the boundary value $W_0(x_0)$ as close to the exact one as possible, we impose the boundary condition as

$$z_n(x_0;x_0)=W_n(x_0)=0 \quad \text{or} \quad Q_n(x_0;x_0)=0, \tag{18}$$

for $n\geqslant 1$.

Since $Q_1(x;x_0)$ satisfies the same equation as $P_1(x)$ does, one readily obtains

$$Q_1(x;x_0)=P_1(x)-P_1(x_0), \tag{19}$$

which satisfies the boundary condition (BC) Eq. (18). Notice that a constant is the solution of the homogeneous equation. The second-order equation now reads

$$Q_2''(x;x_0)-xQ_2'(x;x_0)=\left(\frac{x^4}{4}P_1(x)-\sum_{j=0}^{2}P_j(x)E_{n-j}\right) -P_1(x_0)\left(\frac{x^4}{4}-E_1\right). \tag{20}$$

One can verify that E_2 is given Eq. (9). Since Eq. (20) is linear and the inhomogeneous part is a linear combination of those for $P_2(x)$ and $P_1(x)$, $Q_2(x;x_0)$ is given by a linear combination of $P_2(x)$ and $P_1(x)$:

$$Q_2(x;x_0)=(P_2(x)-P_2(x_0))-P_1(x_0)(P_1(x)-P_1(x_0)), \tag{21}$$

which satisfies the BC $Q_2(x_0;x_0)=0$. One finds that $Q_3(x;x_0)$ satisfies

$$Q_3''(x;x_0)-xQ_3'(x;x_0)=\left(\frac{x^4}{4}P_2(x)-\sum_{j=0}^{3}P_j(x)E_{n-j}\right) -P_1(x_0)\left(\frac{x^4}{4}P_1(x) -\sum_{j=0}^{2}P_j(x)E_{n-j}\right)-[P_2(x_0) -P_1(x_0)^2]\left(\frac{x^4}{4}-E_1\right). \tag{22}$$

One can see that the inhomogeneous part is again composed of a linear combination of those for $P_n(x)$ $(n=1,2,3)$. Thus the solution satisfying the BC is found to be

$$Q_3(x;x_0)=P_3(x)-P_3(x_0)-P_1(x_0)[P_2(x)-P_2(x_0)] -[P_2(x_0)-P_1(x_0)^2][P_1(x)-P_1(x_0)]. \tag{23}$$

We remark that E_3 is the same as that obtained for $P_3(x)$.

Repeating the procedure, one finds that $Q_n(x;x_0)$ are expressed in terms of $P_j(x)$ $(j\leqslant n)$. For instance,

$$Q_4(x;x_0)=P_4(x)-P_4(x_0)-P_1(x_0)[P_3(x)-P_3(x_0)] -[P_2(x_0)-P_1(x_0)^2][P_2(x)-P_2(x_0)] -[P_3(x_0)-2P_1(x_0)P_2(x_0)+P_1(x_0)^3][P_1(x) -P_1(x_0)]. \tag{24}$$

Thus we obtain the approximate solution valid around $x\sim x_0$

$$\psi(x;x_0)\sim A(x_0)e^{-x^2/4}\sum_{n=0}^{\infty}\epsilon^n Q_n(x;x_0), \tag{25}$$

which satisfies the boundary condition

$$\psi(x_0;x_0)=W_0(x_0)=A(x_0)e^{-x_0^2/4}. \tag{26}$$

One may say that now we have obtained a family of curves $\{\psi(x;x_0)\}_{x_0}$ with x_0 parametrizing the curves. If $x_0<x<x_0+\Delta x$ with Δx being sufficiently small, the wave functions $\psi(x;x_0)$ and $\psi(x;x_0+\Delta x)$ should give the same value at x, i.e.,

$$\psi(x;x_0)=\psi(x;x_0+\Delta x). \tag{27}$$

Taking the limit $\Delta x\to 0$ this condition is found to yield that

$$\left.\frac{d\psi(x;x_0)}{dx_0}\right|_{x_0=x}=0. \tag{28}$$

Notice that when $\Delta x\to 0$, $x\to x_0$. This is the basic equation of our method. This is nothing, but the condition to construct the *envelope* of the perturbative wave functions valid around $x\sim x_0$. It is apparent that the equation has the same form as the renormalization group equation, hence the name of the RG method. The equation gives a condition which $A(x_0)$ must satisfy

$$\frac{dA}{dx}=A(x)\frac{d}{dx_0}\sum_{n=0}^{\infty}\epsilon^n(-Q_n(x;x_0))\Bigg|_{x_0=x}. \tag{29}$$

Defining $f_n(x)$ by

$$-\frac{d}{dx_0}Q_n(x;x_0)\Bigg|_{x_0=x}=\frac{df_n(x)}{dx}, \tag{30}$$

one obtains

$$A(x)=\overline{A}\cdot\exp\left[\sum_{n=0}^{\infty}\epsilon^n f_n(x)\right]. \tag{31}$$

With this solution, the global solution $\psi_E(x)$ is given by the boundary value by construction:

$$\psi_E(x)=W_0(x)=A(x)e^{-x^2/4}=\overline{A}\exp\left(-\frac{x^2}{4}+\sum_{n=1}^{\infty}\epsilon^n f_n(x)\right). \tag{32}$$

This is one of the main results of the present paper.

$f_n(x)$'s are easily calculated in terms of $P_n(x)$, and we have

$$f_1(x)=P_1(x)=-\frac{3}{8}x^2-\frac{1}{16}x^4, \tag{33}$$

$$f_2(x)=P_2(x)-\frac{1}{2}P_1(x)^2=\frac{21}{16}x^2+\frac{11}{64}x^4+\frac{1}{96}x^6,$$

$$f_3(x)=P_3(x)-P_1(x)P_2(x)+\frac{1}{3}P_1(x)^3,$$

$$=-\frac{333}{32}x^2-\frac{45}{32}x^4-\frac{21}{192}x^6-\frac{1}{256}x^8,$$

$$f_4(x)=P_4(x)-P_1(x)P_2(x)-\frac{1}{2}P_2(x)^2+P_1(x)^2P_2(x)$$
$$-\frac{1}{4}P_1(x)^4,$$
$$=\frac{30885}{256}x^2+\frac{8669}{512}x^4+\frac{1159}{768}x^6+\frac{163}{2048}x^8+\frac{x^{10}}{512},$$
$$f_5(x)=P_5(x)-P_1(x)P_4(x)-P_2(x)P_3(x)+P_1(x)P_2(x)^2$$
$$-P_1(x)^3P_2(x)+P_1(x)^2P_3(x)+\frac{1}{5}P_1(x)^5,$$
$$=-\frac{916731}{512}x^2-\frac{33171}{128}x^4-\frac{6453}{256}x^6-\frac{823}{512}x^8$$
$$-\frac{319}{5120}x^{10}-\frac{7}{6144}x^{12},$$
$$f_6(x)=P_6(x)-P_1(x)P_5(x)-P_2(x)P_4(x)+P_1(x)^2P_4(x)$$
$$-\frac{1}{2}P_3(x)^2+2P_1(x)P_2(x)P_3(x)-P_1(x)^3P_3(x)$$
$$+\frac{1}{3}P_2(x)^3-\frac{3}{2}P_1(x)^2P_2(x)^2+P_1(x)^4P_2(x)$$
$$-\frac{1}{6}P_1(x)^6,$$
$$=\frac{65518401}{2048}x^2+\frac{19425763}{4096}x^4+\frac{752825}{1536}x^6$$
$$+\frac{43783}{4096}x^8+\frac{3481}{2048}x^{10}+\frac{1255}{24576}x^{12}+\frac{3}{4096}x^{14},$$

and so on. $f_1(x)\sim f_3(x)$ coincide with the results in [6], where explicit expressions of $f_n(x)$ are given only for $n\leqslant 3$. It is interesting that the polynomials $f_n(x)$ are given in terms of $P_n(x)$ appearing in the naive perturbative expansion in a closed form.

Here learned readers may have suspected that $f_i(x)$'s $(i=1,2,3,\ldots)$ are the *cumulant* [11] of the sum $\Sigma_{n=0}^{\infty}\epsilon^n P_n(x)$ in the sense that

$$\sum_{n=0}^{\infty}\epsilon^n P_n(x)\sim\exp\left[\sum_{n=0}^{\infty}\epsilon^n f_n(x)\right]. \tag{34}$$

In fact, this is the case. When a function $C(\xi)$ of ξ is given by $C(\xi)=\Sigma_{n=0}^{\infty}\xi^n/n!\cdot\mu_n$, the nth cumulant λ_n is defined by $\ln C(\xi)=\Sigma_{n=0}^{\infty}\xi^n/n!\cdot\lambda_n$. Expanding $\ln C(\xi)=\ln(1+\xi\mu_1+\xi^2/2\cdot\mu_2+\ldots)$, one finds that $\lambda_1=\mu_1$, $\lambda_2=\mu_2-\mu_1^2$, $\lambda_3=\mu_3-3\mu_1\mu_2+2\mu_1^2$, $\lambda_4=\mu_4-4\mu_1\mu_3-3\mu_2^2+12\mu_1^2\mu_2-6\mu_1^4$, $\lambda_5=24\mu_1^5-60\mu_1^3\mu_2+30\mu_1\mu_2^2+20\mu_1^2\mu_3-10\mu_2\mu_3-5\mu_1\mu_4+\mu_5$, $\lambda_6=-120\mu_1^6+360\mu_1^4\mu_2-270\mu_1^2\mu_2^2+30\mu_2^3-120\mu_1^3\mu_3+120\mu_1\mu_2\mu_3-10\mu_3^2+30\mu_1^2\mu_4-15\mu_2\mu_4-6\mu_1\mu_5+\mu_6$, and so on. Putting $\mu_n=n!P_n$ and $\lambda_n=n!f_n$, one sees that the relation Eq. (33) between P_n and f_n is reproduced. In short, the RG method based on the construction of an envelope certainly resums the perturbation series of the wave function and the resultant expression is given in terms of the cumulants of the naive perturbation series.

Now let us examine how the WKB result Eq. (3) can be constructed from the perturbation series obtained above. Bender and Bettencourt found that if all terms beyond $(1/512)\epsilon^4x^{10}$ are neglected, the sum of the highest power terms in $f_j(x)$ $(j\leqslant 4)$ is nicely rewritten as

$$-\frac{x^2}{4}\left(1+2\epsilon x^2+\frac{17}{12}\epsilon^2x^4+\frac{5}{12}\epsilon^3x^6+\frac{47}{1152}\epsilon^4x^8\right)^{1/8}, \tag{35}$$

which behaves for large x as

$$-\sqrt{\epsilon}|x|^3/4(1152/47)^{1/8}\simeq\sqrt{\epsilon}|x|^3/5.96663 \tag{36}$$

in an excellent agreement with the WKB result. How about the higher orders. In the fifth order, the sum of the highest powers may be rewritten by neglecting all terms beyond $7\epsilon^5x^{10}/1286$ as

$$-\frac{x^2}{4}(1+\epsilon x^2/4-\epsilon^2x^4/24+\epsilon^3x^6/64-\epsilon^4x^8/128$$
$$+7\epsilon^5x^{10}/1286)$$
$$\sim-\frac{x^2}{4}\left(1+\frac{5}{2}\epsilon x^2+\frac{115}{48}\epsilon^2x^4\right.$$
$$\left.+\frac{35}{32}\epsilon^3x^6+\frac{15}{64}\epsilon^4x^8+\frac{4459}{164608}\epsilon^5x^{10}\right)^{1/10}. \tag{37}$$

For large x, the coefficient of $-\sqrt{\epsilon}|x|^3$ is

$$4(164608/4459)^{1/10}\simeq 5.73827, \tag{38}$$

which deviates from 6 more than the fourth-order result. The sixth order becomes worse: The sum of the highest powers is rewritten as

$$-\frac{x^2}{4}\left(1+3\epsilon x^2+\frac{29}{8}\epsilon^2x^4+\frac{9}{4}\epsilon^3x^6+\frac{577}{768}\epsilon^4x^8\right.$$
$$\left.+\frac{67621}{493824}\epsilon^5x^{10}+\frac{1324349}{35555328}\epsilon^6x^{12}\right)^{1/12}, \tag{39}$$

which makes the coefficient of $-\sqrt{\epsilon}|x|^3$ for large x

$$4(35555328/1324349)^{1/12}\simeq 5.26181. \tag{40}$$

In summary, we have successfully applied the RG method as formulated in [3] to the Schrödinger equation of the quantum anharmonic oscillator (AHO): The naive perturbation series of the wave function are resummed by the RG equation. We have seen that the resummation is performed in the RG method more mechanically and explicitly than in MSPT. We have shown that the resummed series $\Sigma_{n=0}^{\infty}\epsilon^n f_n(x)$ is the *cumulant* of the naive perturbation series. We have worked out up to the sixth order in the perturbative expansion and found the following: Although the sum of the highest power in $f_n(x)$ can be organized so that it becomes asymptotically proportional to $\sqrt{\epsilon}|x|^3$ as was done in [6,8], the coefficient of

it reaches the closest value to 6, the WKB result, in the fourth order, then goes away monotonously from the closest value in the higher orders. This is plausible because the convergence radius of the perturbation series is zero; the cumulant series should be at best an asymptotic series. We remark that the RG method as developed here can be also applied to the first excited state; it is, however, unlikely that the method can be used to the higher excited states beyond the first excited state.

We stress that the method presented here can improve perturbative wave functions for all cases where naive perturbative solutions of Bender-Wu type are given. It means that the RG method combined with the Bender-Wu perturbation method constitutes a new powerful method for improving perturbative wave functions. We hope to report on applications of the present method to other quantum systems and on a possible extension to quantum field theory in forthcoming papers; we remark that the amplitude $A(x_0)$ in Eq. (15) corresponds to the wave function renormalization constant.

Finally, we mention that a variational perturbation method called the delta-expansion method [15] has been extended for obtaining wave functions [16]. The key ingredient of the extension is to construct an envelope of a set of perturbative wave functions as in the RG method, but *with a variational parameter*. In this method, although the basic equation can not be solved analytically but only numerically, uniformly valid wave functions with correct asymptotic behavior are obtained in the first-order perturbation even for strong couplings and for excited states. In the present method, the basic equations are solved analytically, and the asymptotic form of the wave function is constructed explicitly, although a further resummation devised in [6,8] is needed for obtaining the asymptotic form. In this sense, the two methods are complementary.

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