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# Perturbative analysis of the ground-state wavefunctions of the quantum anharmonic oscillators

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**Abstract**
We investigate the perturbative expansions of the ground-state wavefunctions of the quantum anharmonic oscillators. With an appropriate change of spatial scale, the weak-coupling Schrödinger equation is transformed to an equivalent strong-coupling one. The Friedberg–Lee–Zhao method is applied to obtain the improved perturbative expansions. These perturbative expansions give a correction to the WKB results for large spatial distances, and reproduce the conventional weak-coupling results for small spatial distances.

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## 1. Introduction

Quantum anharmonic oscillators have now become an important model for testing various approximate methods. For example, they have been used to study conventional Rayleigh–Schrödinger perturbation theory [1], Padé and Borel summation of perturbation series [2], the variational perturbation method [3–6] and strong coupling expansions [7–9]. The list provided here is far from exhaustive. In a series of pioneering works, Bender and Wu have applied the conventional Rayleigh–Schrödinger perturbation theory to present the weak-coupling expansions for the energy eigenvalues and eigenfunctions of quantum anharmonic oscillators. It has been shown that the naive perturbation expansions for the energy eigenvalues are usually divergent. To find the convergent forms of the energy eigenvalues, several other methods have been developed in the past several decades [3–15]. On the other hand, in the conventional perturbation method, the wavefunctions of quantum anharmonic oscillators are generally written as a Gaussian multiplied by a polynomial. By resumming the perturbation series, Bender and Bettencourt have constructed the asymptotic behavior of the wavefunctions for large spatial distances [16]. This asymptotic behavior agrees well with the WKB result. Kunihiro has shown in a subsequent work that the naive perturbation series can be represented by an exponential function [17]. Following the resummation performed by Bender and

  

Bettencourt, the author found that the agreement with the WKB result becomes worse if the higher order terms are included.

In this paper, we reconsider the perturbative expansions of the ground-state wavefunctions of the quantum anharmonic oscillators. With the help of a scaling transformation, we obtain an equivalent strong-coupling Schrödinger equation. The Friedberg–Lee–Zhao (FLZ) method is then applied to obtain a perturbative series of the ground-state wavefunctions [18]. This perturbative series agrees with the WKB results for large spatial distances, and reproduces the conventional weak-coupling results for small spatial distances. In particular, we shall show that the WKB result can be exactly obtained by resumming the highest-power terms in the perturbation expansions given by Kunihiro.

## 2. The ground states of the quantum anharmonic oscillators

We first give a brief introduction to the results given by Bender and Bettencourt and Kunihiro. Following the notations of Bender and Bettencourt, we consider the following Schrödinger equation for the quantum anharmonic oscillators:

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{1}{4}x^2+\frac{1}{4}\epsilon x^{2m}-E\right)\psi(x)=0, m=2,3,4\ldots, \qquad (1)$$

with the boundary condition $\psi(\pm\infty)=0$. Here $0<\epsilon\ll 1$ is the small parameter. In the conventional Rayleigh–Schrödinger perturbation theory, the wavefunction and the eigenvalue for the ground state are both expanded in terms of power series of $\epsilon$ [16]:

$$\psi(x)=\sum_{n=0}^{\infty}\epsilon^n \mathrm{e}^{-\frac{1}{4}x^2}P_n(x), \qquad E=\sum_{n=0}^{\infty}\epsilon^n E_n, \qquad (2)$$

where $P_n(x)$ is a polynomial of degree $2n$ in the variable $x^2$. For $m=2$, Bender and Bettencourt have presented the polynomials $P_n(x)$ up to the sixth order [16]. Kunihiro has further shown that the conventional perturbation expansion can be re-expressed as [17]

$$\mathrm{e}^{-\frac{1}{4}x^2}\sum_{n=0}^{\infty}\epsilon^n P_n(x)=\exp\left[-\sum_{n=0}^{\infty}\epsilon^n f_n(x)\right]. \qquad (3)$$

The polynomials $f_n(x)$ up to the sixth order are listed as follows [17]:

$$\begin{aligned}
f_0(x)&=\frac{1}{4}x^2,\\
f_1(x)&=\frac{3}{8}x^2+\frac{1}{16}x^4,\\
f_2(x)&=-\frac{21}{16}x^2-\frac{11}{64}x^4-\frac{1}{96}x^6,\\
f_3(x)&=\frac{333}{32}x^2+\frac{45}{32}x^4+\frac{7}{64}x^6+\frac{1}{256}x^8,\\
f_4(x)&=-\frac{30\,885}{256}x^2-\frac{8669}{512}x^4-\frac{1159}{768}x^6-\frac{163}{2048}x^8-\frac{1}{512}x^{10},\\
f_5(x)&=\frac{916\,731}{512}x^2+\frac{33\,171}{128}x^4+\frac{6453}{256}x^6+\frac{823}{512}x^8+\frac{319}{5120}x^{10}+\frac{7}{6144}x^{12},\\
f_6(x)&=-\frac{65\,518\,401}{2048}x^2-\frac{19\,425\,763}{4096}x^4-\frac{752\,825}{1536}x^6-\frac{43\,783}{4096}x^8\\
&\quad-\frac{3481}{2048}x^{10}-\frac{1255}{24\,576}x^{12}-\frac{3}{4096}x^{14},
\end{aligned} \qquad (4)$$

where the normalization condition $\psi(0) = 1$ has been used, and we have thus $f_n(0) = 0$. The corresponding energy eigenvalue up to the three-order terms is given by

$$E_0 = \frac{1}{2}, \qquad E_1 = \frac{3}{4}, \qquad E_2 = -\frac{21}{8}, \qquad E_3 = \frac{333}{16}. \tag{5}$$

On the other hand, WKB analysis shows that for large $x$

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

To study how this perturbation expansion can reproduce the WKB behavior, Bender and Bettencourt found that if all terms beyond $\epsilon^4 x^{10}/512$ are neglected, the sum of the highest-power terms in $f_j(x)(j \leqslant 4)$ is nicely rewritten as

$$\frac{x^2}{4}\left(1 + \epsilon x^2 + \frac{17}{12}\epsilon^2 x^4 + \frac{5}{12}\epsilon^3 x^6 + \frac{77}{1152}\epsilon^4 x^8\right)^{1/8}, \tag{7}$$

which behaves for large $x$ as

$$\frac{\sqrt{\varepsilon}|x|^3}{4(1152/77)^{1/8}} \simeq \frac{\sqrt{\varepsilon}|x|^3}{5.966\,63}. \tag{8}$$

This result has an excellent agreement with the WKB result. However, Kunihiro found that by neglecting all terms beyond $7\epsilon^5 x^{12}/6144$, the sum of the highest powers in $f_j(x)(j \leqslant 5)$ may be rewritten as

$$\frac{x^2}{4}\left(1 + \frac{5}{2}\epsilon x^2 + \frac{115}{48}\epsilon^2 x^4 + \frac{35}{32}\epsilon^3 x^6 + \frac{15}{64}\epsilon^4 x^8 + \frac{4459}{164\,608}\epsilon^5 x^{10}\right)^{1/10}. \tag{9}$$

For large $x$, its asymptotic behavior is

$$\frac{\sqrt{\varepsilon}|x|^3}{4(164\,608/4459)^{1/10}} \simeq \frac{\sqrt{\varepsilon}|x|^3}{5.738\,27}. \tag{10}$$

When the sixth order is included by neglecting all terms beyond $3\epsilon^6 x^{14}/4096$, the sum of the highest powers in $f_j(x)(j \leqslant 6)$ is rewritten as

$$\frac{x^2}{4}\left(1 + 3\epsilon x^2 + \frac{29}{8}\epsilon^2 x^4 + \frac{9}{4}\epsilon^3 x^6 + \frac{577}{768}\epsilon^4 x^8 + \frac{67\,621}{493\,824}\epsilon^5 x^{10} + \frac{1324\,349}{35\,555\,328}\epsilon^6 x^{12}\right)^{1/12}, \tag{11}$$

where the coefficient of $\sqrt{\epsilon}|x|^3$ for large $x$ is given by

$$\frac{1}{4(35\,555\,328/1324\,349)^{1/12}} \simeq \frac{1}{5.261\,81}. \tag{12}$$

It follows from the above results that the agreement with the WKB result becomes worse when higher order terms are included, and thus is the best at the fourth order [17]. In the following, we shall show that the sum of the highest-power terms in $f_j(x)$ can exactly reproduce the WKB behavior.

With the change of variable $z = \epsilon^{\frac{1}{2(m-1)}} x$, the Schrödinger equation (1) can be transformed into an equivalent strong-coupling Schrödinger equation

$$\left[-\frac{d^2}{dz^2} + \frac{g^2}{4}(z^2 + z^{2m}) - \widetilde{E}(g)\right]\psi(z) = 0, \tag{13}$$

where $g = \epsilon^{1/(1-m)} \gg 1$ and $\widetilde{E}(g) = E/g$. For the ground state, the wavefunction can be written as

$$\psi(z) = e^{-S(z)}, \tag{14}$$

and then $S(z)$ has to satisfy

$$\frac{d^2S}{dz^2} - \left(\frac{dS}{dz}\right)^2 + \frac{g^2}{4}(z^2 + z^{2m}) - \widetilde{E}(g) = 0. \tag{15}$$

In the case of large $g$, Friedberg, Lee and Zhao have proposed the following expansions in terms of $g$ for $S$ and $\widetilde{E}$ [18]:

$$S(z) = \sum_{n=0}^{\infty} g^{1-n} S_n(z), \tag{16}$$

$$\widetilde{E}(g) = \sum_{n=0}^{\infty} g^{1-n} \widetilde{E}_n. \tag{17}$$

Substituting equations (16) and (17) into equation (15), and equating the coefficients of like powers of $g$ on both sides, we find equations for successive determination of $S_n$ and $\widetilde{E}_n$:

$$-\left(\frac{dS_0}{dz}\right)^2 + \frac{1}{4}z^2 + \frac{1}{4}z^{2m} = 0, \tag{18}$$

$$\frac{d^2S_{n-1}}{dz^2} - 2\frac{dS_0}{dz}\frac{dS_n}{dz} - \sum_{k=1}^{n-1}\frac{dS_k}{dz}\frac{dS_{n-k}}{dz} - \widetilde{E}_{n-1} = 0 \quad (n \geqslant 1). \tag{19}$$

If we adopt the normalization condition $\psi(0) = 1$, we require $S_n(0) = 0$. From equation (18), one can obtain $S_0$, and then substitute it into equation (19) with $n = 1$. By requiring $S_1$ to be analytic at $z = 0$, we can obtain $\widetilde{E}_0$ and then $S_1$. In such a way, one can determine all $\widetilde{E}_n$ and $S_n$. In what follows, for brevity, we shall only consider the following two cases: $m = 2$ and $m = 3$.

### 2.1. The case of $m = 2$

In the case of $m = 2$, we have $z = \sqrt{\epsilon}x$ and $g = 1/\epsilon$. It follows from equation (18) that

$$\frac{dS_0}{dz} = \frac{\sqrt{z^2 + z^4}}{2}, \tag{20}$$

where due to the boundary condition $\psi(\pm\infty) = 0$, we take the positive square root. $S_0(z)$ is thus given by

$$S_0(z) = \tfrac{1}{6}\left[(1 + z^2)^{3/2} - 1\right]. \tag{21}$$

Substituting $S_0(z)$ into equation (19) with $n = 1$ yields

$$\frac{dS_1}{dz} = \frac{1 + 2z^2}{2(z + z^3)} - \frac{\widetilde{E}_0}{\sqrt{z^2 + z^4}}. \tag{22}$$

For $S_1$ to be analytic at $z = 0$, we require that the limit

$$\lim_{z\to 0} \frac{1 + 2z^2 - 2\widetilde{E}_0\sqrt{1 + z^2}}{2(z + z^3)} \tag{23}$$

should be a finite value. This leads to $\widetilde{E}_0 = 1/2$ and

$$S_1(z) = \frac{1}{4}\left[\ln(1 + z^2) + 2\ln\left(1 + \sqrt{1 + z^2}\right) - 2\ln 2\right]. \tag{24}$$

After substitution of $S_0(z)$ and $S_1(z)$ into equation (19) with $n = 2$, we have

$$\frac{dS_2}{dz} = \frac{1}{4z^3(1 + z^2)^{5/2}}\left[-4 - 7z^2 - 8z^4 + (4 + 8z^2)\sqrt{1 + z^2} - 4\widetilde{E}_1 z^2(1 + z^2)^2\right]. \tag{25}$$

For $S_2$ to be analytic at $z = 0$, we obtain $\widetilde{E}_1 = 3/4$ and

$$S_2(z) = \frac{1}{12z^2(1+z^2)^{3/2}}\left[6 + 20z^2 + 9z^4 - (6 + 17z^2 + 17z^4)\sqrt{1+z^2}\right]. \tag{26}$$

In a similar way, one can determine all $\widetilde{E}_n$ and $S_n$.

In the following, we discuss the asymptotic behavior for the ground-state wavefunction. As $z \to \pm\infty$, we have

$$S_0(z) \to \frac{1}{6}|z|^3, \tag{27}$$

$$S_1(z) \to \ln|z|, \tag{28}$$

$$S_2(z) \to -\frac{17}{12}. \tag{29}$$

It is clearly seen that for large $x$, $gS_0 \to \sqrt{\epsilon}|x|^3/6$ corresponds to the WKB result, and $S_1 \to \ln|\sqrt{\epsilon}x|$ represents its correction. Due to $|x|^3 \gg \ln|x|$ for large $x$, the asymptotic behavior of the wavefunction is mainly determined by $\exp\left(-\sqrt{\epsilon}|x|^3/6\right)$. We note that as $x \to \pm\infty$, $S_2(x)$ approaches a finite value of $-17/12$. This motivates us to continue our calculations. With higher order calculations, we further find that such a behavior also appears in $S_n(n \geqslant 3)$ indeed. It follows that the WKB method provides a very accurate analysis of the asymptotic behavior of the ground-state wavefunction for large $x$.

For small $z$, we can have the following expansions:

$$S_0(z) = \frac{1}{4}z^2 + \frac{1}{16}z^4 - \frac{1}{96}z^6 + \frac{1}{256}z^8 - \frac{1}{512}z^{10} + \frac{7}{6144}z^{12} - \frac{3}{4096}z^{14} + \cdots, \tag{30}$$

$$S_1(z) = \frac{3}{8}z^2 - \frac{11}{64}z^4 + \frac{7}{64}z^6 - \frac{163}{2048}z^8 + \frac{319}{5120}z^{10} - \frac{1255}{24576}z^{12} + \cdots, \tag{31}$$

$$S_2(z) = -\frac{21}{16}z^2 + \frac{45}{32}z^4 - \frac{1159}{768}z^6 + \frac{823}{512}z^8 - \frac{3481}{2048}z^{10} + \cdots. \tag{32}$$

With equations (4) and (30), we observe that $gS_0(z)$ is the total sum of the highest-power terms in $\epsilon^j f_j(x)(j \geqslant 0)$. This result can be verified by using the relation $\sum_{n=0} g^{1-n}S_n(z) = \sum_{n=0}\epsilon^n f_n(x)$. Due to $z = \sqrt{\epsilon}x$ and $g = 1/\epsilon$, the highest-power terms in $\epsilon^j f_j(x)$ are $\sim gz^{2j+2}$, and $S_0$ is thus the collection of the terms with the same order of $g$. Similarly, $S_1$ is the sum of the second highest-power terms in $\epsilon^j f_j(x)(j \geqslant 0)$ behaving as $z^{2j}$ for small $x$. Clearly, our perturbation expansion actually corresponds to a resummation of the perturbation expansion given by Kunihiro.

On the other hand, the conventional weak-coupling expansion for the energy eigenvalue can be obtained from our perturbative expansion by the relation

$$\sum_{n=0} g^{1-n}\widetilde{E}_n = \sum_{n=0}\epsilon^n \overline{E}_n. \tag{33}$$

Therefore, in a comparison with equation (2), we find that the FLZ method gives the same perturbative expansion for the energy eigenvalue with the conventional perturbation theory.

*2.2. The case of $m = 3$*

In the case of $m = 3$, we have $z = \epsilon^{1/4}x$ and $g = \epsilon^{-1/2}$. $S_n(z)'s$ up to the three-order terms are given by

$$S_0(z) = \frac{1}{8}\left[z^2\sqrt{1+z^4} + \text{arcsinh} z^2\right], \tag{34}$$

$$S_1(z) = \frac{1}{4}\left[\ln(1+z^4) + \ln\left(1+\sqrt{1+z^4}\right) - \ln 2\right], \tag{35}$$

$$S_2(z) = \frac{1}{24z^2\left(1+z^4\right)^{3/2}}\left[12 + 51z^4 + 19z^8 - 12\sqrt{1+z^4}\right], \tag{36}$$

$$S_3(z) = \frac{1}{8z^4\left(1+z^4\right)^3}\Big[-10 - 55z^4 - 195z^8 - 165z^{12} - 55z^{16} + (10 + 50z^4 + 35z^8 + 15z^{12})\sqrt{1+z^4}\Big]. \tag{37}$$

As $z \to \pm\infty$, we have

$$S_0(z) \to \frac{1}{8}z^4, \tag{38}$$

$$S_1(z) \to \ln|z|, \tag{39}$$

$$S_2(z) \to \frac{19}{24}, \tag{40}$$

$$S_3(z) \to -\frac{55}{8}. \tag{41}$$

In this case, we find that as $x \to \pm\infty$, $S_n(x)(n \geqslant 2)$ approaches a finite value. Therefore, $gS_0 \to \sqrt{\epsilon}x^4/8$ corresponds to the WKB result, and $S_1 \to \ln|\epsilon^{1/4}x|$ is its correction. With $z = \epsilon^{1/4}x$ and $g = \epsilon^{-1/2}$, the highest-power terms of $\epsilon^j f_j(x)$ for small $x$ are $\sim gz^{4j+2}$. The sum of all the terms with the same order of $g$ leads to $gS_0(z)$. The second highest-power terms of $\epsilon^j f_j(x)$ for small $x$ are $\sim z^{4j}$, and the sum of them is $S_1$. Generally, $g^{1-n}S_n$ is the sum of the $n$th highest-power terms in $\epsilon^j f_j(x)(j \geqslant n)$. In addition, with $\sum_{n=0} g^{1-n}S_n(z) = \sum_{n=0}\epsilon^n f_n(x)$ for small $x$, we can obtain the polynomials $f_n(x)$. Here we only present them up to the third order:

$$f_0(x) = \frac{1}{4}x^2, \tag{42}$$

$$f_1(x) = \frac{15}{8}x^2 + \frac{5}{16}x^4 + \frac{1}{24}x^6, \tag{43}$$

$$f_2(x) = -\frac{3495}{32}x^2 - \frac{545}{32}x^4 - \frac{47}{24}x^6 - \frac{19}{128}x^8 - \frac{1}{160}x^{10}, \tag{44}$$

$$f_3(x) = \frac{1239\,675}{64}x^2 + \frac{197\,875}{64}x^4 + \frac{72\,385}{192}x^6 + \frac{2165}{64}x^8 + \frac{141}{64}x^{10} + \frac{37}{384}x^{112} + \frac{1}{448}x^{14}. \tag{45}$$

These expressions can also be obtained directly by the exponential perturbation theory [17].

On the other hand, the ground energy up to the three-order terms is given by

$$\widetilde{E}_0 = \frac{1}{2}, \qquad \widetilde{E}_1 = 0, \qquad \widetilde{E}_2 = \frac{15}{4}, \qquad \widetilde{E}_3 = 0. \tag{46}$$

With $\sum_{n=0} g^{1-n}\widetilde{E}_n = \sum_{n=0} \epsilon^{n/2}\overline{E}_n$, we can obtain the relation between the conventional weak-coupling expansion and our perturbative expansion: $E_n = \overline{E}_{2n}$. For example, $E_0 = \widetilde{E}_0 = 1/2$ and $E_1 = \widetilde{E}_2 = 15/4$ are just the first two terms in the conventional perturbation expansion.

## 3. Conclusion

In conclusion, by using a simple scaling transformation, we have transformed the original weak-coupling Schrödinger equation to an equivalent strong-coupling one. This allows us to apply the FLZ method to obtain the perturbative expansions for the ground states of the quantum anharmonic oscillators. It is shown that although we cannot obtain a better perturbative expansion for the energy eigenvalues, we can get an improved wavefunction of the ground state, which agrees with the WKB result for large spatial distances, and gives the conventional weak-coupling result for small spatial distances. Our perturbative expansion corresponds to resumming the exponential perturbation expansion given by Kunihiro. The correction to the WKB result is also presented. In particular, we show that the sum of the highest-power terms in the exponential perturbation expansion can reproduce the well-known WKB results.

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## References

[1] Bender C M and Wu T T 1968 *Phys. Rev. Lett.* **21** 406
Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
Bender C M and Wu T T 1971 *Phys. Rev. Lett.* **27** 461
Bender C M and Wu T T 1973 *Phys. Rev.* D **7** 1620
[2] Simon B 1970 *Ann. Phys.* **58** 76
[3] Bazley N and Fox D 1961 *Phys. Rev.* **124** 483
[4] Reid C 1965 *J. Chem. Phys.* **43** 186
[5] Graffi S and Grecchi V 1973 *Phys. Rev.* D **8** 3487
[6] Hatsuda T, Kunihiro T and Tanaka T 1997 *Phys. Rev. Lett.* **78** 3229
[7] Vinette F and Čížek J 1991 *J. Math. Phys.* **32** 3392
[8] Weniger E J, Čížek J and Vinette F 1993 *J. Math. Phys.* **34** 571
Weniger E J 1996 *Ann. Phys.* **246** 133
Weniger E J 1996 *Phys. Rev. Lett.* **77** 2859
[9] Janke W and Kleinert H 1995 *Phys. Rev. Lett.* **75** 2787
[10] Biswas S N, Datta K, Saxena R P, Srivastava P K and Verma V S 1973 *J. Math. Phys.* **14** 190
[11] Killingbeck J 1980 *J. Phys. A: Math. Gen.* **13** 49
[12] Jing-Ling C, Kwek L C, Oh C H and Yong L 2001 *J. Phys. A: Math. Gen.* **34** 8889
[13] Bhattacharya R, Roy D and Bhowmick S 1998 *Phys. Lett.* A **244** 9
Dasgupta A, Roy D and Bhattacharya R 2007 *J. Phys. A: Math. Theor.* **40** 773
[14] Fernández F M 1994 *Phys. Lett.* A **194** 343
[15] Fernandez F M and Castro E A 1987 *J. Phys. A: Math. Gen.* **20** 5541

[16] Bender C M and Bettencourt A M L 1996 *Phys. Rev. Lett.* **77** 4114
Bender C M and Bettencourt A M L 1996 *Phys. Rev.* D **54** 7710
[17] Kunihiro T 1998 *Phys. Rev.* D **57** R2035
[18] Friedberg R, Lee T D and Zhao W Q 1999 *Il Nuovo Cimento* A **112** 1195
Friedberg R, Lee T D and Zhao W Q 2001 *Ann. Phys.* **288** 52