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The Quantum Anharmonic Potential with the Linear Delta Expansion

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THE QUANTUM ANHARMONIC POTENTIAL WITH THE LINEAR DELTA EXPANSION

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THE QUANTUM ANHARMONIC POTENTIAL WITH THE LINEAR DELTA EXPANSION

by

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REPORT

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Gracias madre por tu eterna ayuda y paciencia durante toda mi vida.

ABSTRACT

In this report the problem of solving the Schrödinger equation for an anharmonic potential is treated using the technique known as the linear delta expansion. The method works by identifying three different scales in the problem: an asymptotic scale, which depends uniquely on the form of the potential at large distances; an intermediate scale, still characterized by an exponential decay of the wavefunction; and, finally, a short distance scale, in which the wavefunction is sizable. The method is found to be suitable to obtain both energy eigenvalues and wavefunctions.

Contents

6

List of Figures

Chapter 1

INTRODUCTION

Subatomic particles trapped in potentials are bound to have specific values of the energy, and their behavior inside the well described by a set of denumerable wavefunctions. These *eigenenergies* and *eigenfunctions* are obtained by solving the Schrödinger equation for the proposed potential; unfortunately, this valuable information can only be obtained exactly for a few specific potentials and, in most realistic cases, one must resort to perturbative methods or numerical solutions.

The most commonly used method, Rayleigh-Schrödinger perturbative expansion, usually generates divergent asymptotic series [1], and thus improvements on the standard perturbative expansion have been proposed in the past (see, e.g., [2, 3, 4, 5, 6] and references therein). These efforts, however, are limited in practice by the complexity of the corrections beyond the first few orders in the perturbative expansion.

Recently, a novel method that works equally well for eigenenergies and eigenfunctions has been proposed [7, 8]. This method, based on the so-called linear delta expansion (LDE) [16]–[30], improves accuracy by correcting the perturbative expansion by means of solving algebraic equations.

The LDE has been extensively applied to, for example, disordered systems [31], the slow roll potential in inflationary models [32], BoseEinstein condensation problem [33], the $O(N)(\phi^2)_{3d}^2$ model [34], the Walecka model [35], and to the ϕ^4 theory at high temperature [36]. More recently, the LDE has been applied with success to the study of classical nonlinear systems [37, 38].

In this report the method is applied to the quantum anharmonic oscillator (AHO). This case has been studied by several perturbative and non-perturbative methods [3, 4, 5, 6, 12, 13, 14, 15].

The report is organized as follows. In chapter 2 the method is introduced. Next, in chapter 3, the method is applied to the quantum anharmonic oscillator and results are presented. Finally, in chapter 4, conclusions are drawn.

Chapter 2

The Linear Delta Expansion

2.1 Introduction

The problem at hand is the solution of the Schrödinger equation with a quartic anharmonic potential of the form $V(x) = m\omega^2 x^2/2 + \mu x^4/2$:

$$
\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2}{2} x^2 + \frac{\mu}{4} x^4 \right] \psi_n(x) = E_n \psi_n(x)
$$
 (2.1)

where m is the mass of the particle, ω the angular frequency, μ the anharmonic coupling, and $\psi_n(x)$ and E_n the eigenfunction and eigenenergy of the n^{th} excited state.

A thorough analysis of this problem is given in [5], but here a different path is followed. First, just like in the multiple-scale perturbation theory [9, 10, 11], a suitable ansatz for the wavefunction will be drafted by identifying different length scales in the problem, and, then, it will be used to generate an optimized perturbative expansion.

The expansion will be obtained within the method known as the *linear delta*

expansion (LDE) [16, 17, 18, 19, 30], and the optimization will be performed by means of the *principle of minimum sensitivity* (PMS) [41].

The LDE has been extensively applied to quantum [31, 32, 33, 34, 35, 36] and classical systems [37, 38]. At a difference from most of these applications, in this work, the LDE is used in a non–canonical way. In most previous applications of the LDE, a Hamiltonian is generically rearranged as:

$$
H = \frac{p^2}{2m} + V(q) \rightarrow H_\delta = H_0 + \delta H'
$$
\n(2.2)

with $H_0 = p^2/2m + \mu x^4/4$ and $H' = V(x) - \mu x^4/4$ with $V(x) = m\omega^2 x^2/2$; so that $H_{\delta=1} \equiv H$. Next, physical quantities are expanded in δ , which is then set equal to 1. Although this yields an expansion with μ -dependent terms, the expansion can be optimized by using the principle of minimal sensitivity on a given observable, say the energy, to determine the most appropriate μ .

Here this method is modified by introducing the trial parameter of the LDE not in the potential of the Hamiltonian, but into the wavefunction. The first step of this approach consists in the identification of three different scales in the problem: large distances (asymptotic behavior determined by the anharmonic potential), intermediate distances (exponential decay governed by harmonic term), and short distances (wavefunction is sizable). After this division of the wavefunction, an arbitrary parameter is introduced in the last two scales to implement the LDE. The optimization of the perturbative expansion through the PMS is then performed over a suitable parameter.

2.2 The Linear Delta Expansion

In this section the linear delta expansion will be used on the wavefunction. First three different scales will be identified in the problem and the wavefunction will be designed accordingly. Next, an arbitrary parameter will be introduced in the wavefunction to implement the linear delta expansion. Finally, the resulting perturbative expansion will be optimized through the use of the principle of minimum sensitivity over a chosen parameter.

2.2.1 The Ansatz for the Wavefunction

Although one cannot solve the Schrödinger equation (2.1) exactly, it is possible to infer the behavior of $\psi_n(x)$ in the different regions. At short distances, where the quartic terms is negligible, equation (2.1) resembles the Hamiltonian of a quadratic potential and, thus, its solution should approximate the Hermite polynomials.

At large x , on the other hand, the equation is dominated by the quartic term and the wavefunction should be a decreasing exponential of some sort. It is possible to extract the asymptotic behavior of $\psi_n(x)$ in the region of large x by substituting the ansatz $\psi_n(x) \propto e^{-\gamma |x|^p}$ into equation (2.1). One obtains $\gamma = (\sqrt{\mu m/2})/3\hbar$ and $p=3$.

Thus, the three scales can be made explicit in the wave function by writing [8]

$$
\psi_n(x) = e^{-\gamma |x|^3 - \beta x^2} \xi_n(x).
$$
\n(2.3)

The exponentials yield the correct behavior in the limit $|x| \to \infty$, the quadratic term in the exponential dominates at scales where $|x| < \beta/\gamma$, and ξ_n is a function which satisfies the equation (2.4) below. Here $\beta = m$ √ $\omega^2 + \Omega^2/2\hbar$ is the coefficient of a

harmonic oscillator of frequency $\tilde{\Omega} \equiv \sqrt{\ }$ $\omega^2 + \Omega^2$, where Ω is an arbitrary parameter. ξ_n satisifies:

$$
\xi_n''(x) - \left[\frac{\sqrt{2m\mu}}{\hbar}x^2 + \frac{2m\tilde{\Omega}x}{\hbar}\right]\xi_n'(x) \tag{2.4}
$$
\n
$$
+ \left[\frac{\sqrt{2\mu m^3\tilde{\Omega}^2}}{\hbar^2}x^3 + \frac{m^2\Omega^2}{\hbar^2}x^2 - \frac{\sqrt{2\mu m}}{\hbar}x + \frac{2mE_n}{\hbar^2} - \frac{m\tilde{\Omega}}{\hbar}\right]\xi_n(x) = 0.
$$

In this way, equation (2.3) is divided into three different regimes which, in turn, simplifies the creation of a perturbative expansion.

The behavior of the wavefunction on each of these regions can be analyzed separately. In the asymptotic regime ($|x| \to \infty$) the cubic term in the exponential dominates; the intermediate regime $|x|$ is large enough to expect the wavefunction to be exponentially damped; in the regime of small $x \mid$ the physics is contained in the ξ . The last two regimes have a dependence on the arbitrary frequency Ω , and the intermediate regime displays a non-perturbative dependence upon Ω . The limit $(\mu,\Omega) \to 0$ yields an equation for the harmonic oscillator of frequency ω , with solutions of the form of the Hermite polynomials [8].

As expected, both the function, $\psi_n(x)$, and the energy, E_n , depend on the anharmonic coefficient μ . On the other hand, they also have a fictitious dependence (*i.e.* not in the original equation (2.1)) on the arbitrary frequency $Ω$. This dependence will be used to produce an expansion for the solution of equation (2.1) .

2.2.2 The Linear Delta Expansion

To produce an expansion, equation (2.4) is first modified by introducing a parameter δ , to be used as a power-counting device:

$$
\xi''_n(x) - \left[\frac{2m\tilde{\Omega}x}{\hbar}\right] \xi'_n(x) + \left[\frac{2mE_n}{\hbar^2} - \frac{m\tilde{\Omega}}{\hbar}\right] \xi_n(x) \tag{2.5}
$$
\n
$$
= \delta \left\{\frac{\sqrt{2\mu m}}{\hbar}x^2\xi'_n(x) - \left[\frac{\sqrt{2\mu m^3\tilde{\Omega}^2}}{\hbar^2}x^3 + \frac{m^2\Omega^2}{\hbar^2}x^2 - \frac{\sqrt{2\mu m}}{\hbar}x\right] \xi_n(x)\right\}.
$$

The effect of the parameter δ disappears when $\delta = 1$: equation (2.5) reduces exactly to (2.4). Notice that the left-hand side of equation (2.5) corresponds to a harmonic oscillator of frequency $\tilde{\Omega}$, with $\xi_n = \exp[-(m\tilde{\Omega}/2\hbar)x^2]$.

Even though δ is not a small parameter, it can now be used to produce a perturbative expansion. Using the expansions

$$
\xi_n(x) = \sum_{j=0}^{\infty} \delta^j \xi_{nj}(x) \qquad E_n = \sum_{j=0}^{\infty} \delta^j E_{nj} \tag{2.6}
$$

on equation (2.5), a hierarchy of equations, corresponding to the different orders in δ, can be generated and used to obtain approximations to $\xi_n(x)$ and E_n .

2.2.3 The Principle of Minimum Sensitivity

The results produced by (2.6) will depend on the arbitrary frequency Ω introduced in (2.4). These results can be optimized by eliminating this dependence; this is achieved through the principle of minimum sensitivity (PMS).

Since the dependence on Ω is fictitious, *i.e.* it did not exist in the original Schrödinger equation, it must be eliminated. This can be done by requiring that a given observable $\mathcal O$ (the energy, for example) be locally independent of Ω :

$$
\frac{\partial \mathcal{O}}{\partial \Omega} = 0. \tag{2.7}
$$

This, in essence, is the principle of minimum sensitivity.

Chapter 3

Results

Now the procedure outlined before is illustrated explicitly up to order one, and results are also presented for higher orders.

3.1 Order Zero

To lowest order (*i.e* to δ^{0}) the expansions reduce to

$$
\xi_n(x) = \xi_{n0}(x) \qquad E_n = E_{n0} \,, \tag{3.1}
$$

and the equation (2.5) to

$$
\xi_{n0}''(x) - \left[\frac{2m\tilde{\Omega}x}{\hbar}\right]\xi_{n0}'(x) + \left[\frac{2mE_n}{\hbar^2} - \frac{m\tilde{\Omega}}{\hbar}\right]\xi_{n0}(x) = 0 \tag{3.2}
$$

As this is the equation for the harmonic oscillator of frequency ω , the solutions ξ_{n0} correspond to the Hermite polynomials $\xi_{n0}(x) = H_n(x)$ $\sqrt{m\tilde{\Omega}}$ $\frac{d\Omega}{h}(x)$ with eigenvalues given by $E_{n0} = \hbar \tilde{\Omega} (n + 1/2)$ with $n = 0, 1, 2, \cdots$

3.2 Order One

To next order (*i.e.* to δ^1) the expansions are:

$$
\xi_n(x) = \xi_{n0}(x) + \delta \xi_{n1}(x) \qquad E_n = E_{n0} + \delta E_{n1} \tag{3.3}
$$

with $\xi_{n0}(x) = H_n(x)$ $\sqrt{m\tilde{\Omega}}$ $\frac{n\tilde{\Omega}}{h}(x)$ and $E_{n0} = \hbar \tilde{\Omega}(n+1/2)$ with $n = 0, 1, 2, \cdots$. Extracting the term proportional to δ^1 from equation (2.5) yields:

$$
\xi_{n1}''(x) - \left[\frac{2m\tilde{\Omega}x}{\hbar}\right] \xi_{n1}'(x) + \frac{2m\tilde{\Omega}}{\hbar} n \xi_{n1}(x) \tag{3.4}
$$
\n
$$
= \left\{-\frac{2mE_{n1}}{\hbar^2} + \frac{\sqrt{2\mu m}}{\hbar}x - \frac{m^2\Omega^2}{\hbar^2}x^2 - \frac{\sqrt{2\mu m^3 \tilde{\Omega}^2}}{\hbar^2}\right\} x^3 \xi_{n0}(x).
$$

Again, $n = 0, 1, 2, \cdots$ denotes the different excited states of the system.

3.2.1 Ground State ξ_0 and E_0 to Order One

The eigenfunctions and eigenvalues can be obtained to $\mathcal{O}(\delta^1)$ from equations (3.2) and (3.4). Equation (3.2) simply yields:

$$
\xi_{00}(x) = 1 \qquad E_{00} = \frac{1}{2}\hbar\tilde{\Omega} \;, \tag{3.5}
$$

but solving equation (3.4) for $\xi_{01}(x)$ and E_{01} on the other hand, is a bit more complicated. Given that equation (3.4) has terms up to x^3 , one could try a solution of the form

$$
\xi_{01}(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3. \tag{3.6}
$$

$$
\left\{ a_1 = 0, \ a_2 = \frac{m\Omega^2}{4\hbar\tilde{\Omega}}, \ a_3 = \frac{1}{3\hbar} \sqrt{\frac{m\mu}{2}} \right\} \Rightarrow \xi_{01}(x) = \frac{m\Omega^2}{4\hbar\tilde{\Omega}} x^2 + \frac{1}{3\hbar} \sqrt{\frac{m\mu}{2}} x^3, \quad (3.7)
$$

and the 1^{st} order contribution to the ground–state eigenenergy is found to be

$$
E_{01} = -\frac{\hbar\Omega^2}{4\tilde{\Omega}}.\tag{3.8}
$$

Thus, the total ground–state eigenfunction and eigenenergy evaluated up to 1^{st} order are

$$
\xi_0^{(1)}(x) = \xi_{00}(x) + \xi_{01}(x) = 1 + \frac{m\Omega^2}{4\hbar\tilde{\Omega}}x^2 + \frac{1}{3\hbar}\sqrt{\frac{m\mu}{2}}x^3.
$$
 (3.9)

and

$$
E_0^{(1)} = E_{00} + E_{01} = \frac{1}{2}\hbar\tilde{\Omega} - \frac{\hbar\Omega^2}{4\tilde{\Omega}}.
$$
\n(3.10)

To evaluate these results it is necessary to know what Ω is, this can be obtained by means of the principle of minimum sensitivity.

3.2.2 Applying the PMS

As predicted in the previous chapter, the results (3.9) and (3.10) depend on the arbitrary frequency Ω , this dependence will be now eliminated through the principle of minimum sensitivity.

To continue with the illustration, the PMS will be applied to the ground state Energy, $E_0^{(1)}$ ⁽¹⁾. Remembering that harmonic oscillator frequency is $\tilde{\Omega} \equiv \sqrt{\frac{2}{\pi}}$ $\omega^2+\Omega^2,$

where Ω is the arbitrary parameter, PMS implies that

$$
\frac{\partial E_0^{(1)}}{\partial \Omega} = \frac{\partial E_0^{(1)}}{\partial \tilde{\Omega}} \frac{\partial \tilde{\Omega}}{\partial \Omega} = \frac{\Omega}{\tilde{\Omega}} \frac{\partial E_0^{(1)}}{\partial \tilde{\Omega}} \n= \frac{\Omega}{\tilde{\Omega}} \frac{\partial (\hbar \tilde{\Omega})}{\partial \Omega} - \frac{\Omega}{\tilde{\Omega}} \frac{\partial (\hbar \Omega^2 / 4\tilde{\Omega})}{\partial \Omega} = \frac{\hbar \Omega^2}{2\tilde{\Omega}^2} + \frac{\Omega^4}{\tilde{\Omega}^4} - \frac{2\Omega^2}{\tilde{\Omega}^2} = 0.
$$
\n(3.11)

which leads immediately to $\Omega = 0$, and to

$$
E_0^{(1)}|_{PMS} = \left\{ \frac{1}{2}\hbar\tilde{\Omega} - \frac{\hbar\Omega^2}{4\tilde{\Omega}} \right\}_{\Omega=0} = \frac{\hbar\omega}{2}.
$$
 (3.12)

which is the expected result for the ground-state energy of the quadratic potential.

3.3 Order Three

To illustrate the fact the higher orders yield improved results, the expression for the energy up to third order is shown next, full details can be obtained through the use of the codes included in the appendix 5.1.1, or can be found in reference [39].

3.3.1 Ground State Energy to Order Three

To third order, *i.e.* to δ^3 , the ground state energy is given by

$$
E_0^{(3)} = \frac{\hbar}{32m^2\tilde{\Omega}^5} \left[6\mu\hbar \tilde{\Omega}(-\omega^2 + 2\tilde{\Omega}^2) + m^2(\omega^6 - 5\omega^4\tilde{\Omega}^2 + 15\omega^2\tilde{\Omega}^4 + 5\tilde{\Omega}^6) \right].
$$
 (3.13)

Again, the Ω can be fixed from the *PMS*, which in this case, for $\hbar = \omega = m = 1$ yields

$$
\frac{\partial E_0^{(3)}}{\partial \Omega} = 0 \quad \Rightarrow \quad \Omega = 2\left(\frac{3\mu}{5}\right)^{1/3} + \mathcal{O}(\mu^{-1/3}),\tag{3.14}
$$

which, in turn yields

$$
E_0^{(3)} = \frac{3}{16} \left(\frac{75\mu}{8}\right)^{1/3} + \mathcal{O}(\mu^{-1/3}) \tag{3.15}
$$

Even though these results are not given in full detail, their derivation, with the use of *Mathematica*, is much easier than their reproduction in *Latex* in this thesis. The proceeding chapter presents results of this procedure extended to much higher orders.

3.4 Higher Orders

The previous procedure can be repeated both for higher orders of δ and for higher energy states. Appendices $5.1.2$ and $5.1.3$ list the *Mathematica* codes used to evaluate the wavefunctions for the 1st excited state up to orders δ^3 and δ^3 , *i.e.* $\psi_1^{(3)}$ $y_1^{(3)}(x)$ and $y_1^{(5)}$ $1^{(5)}(x).$

Chapter 4

Conclusions

Chapter 5

Appendix

5.1 Computer codes

5.1.1 Eigenenergy of ground state to order δ^3

The *Mathematica* code to evaluate the eigenenergy of the ground state to order δ^3 , *i.e.* $E_0^{(3)}$ $C_0^{(3)}(x)$ is $ColimaO(3).nb,$

ξ and E_n to order δ^3

<< Calculus'DSolveIntegrals'

```
SetAttributes[m, Constant];
\texttt{SetAttributes[h, Constant]; SetAttributes[\textit{w, Constant}];}\texttt{SetAttributes}[\mu, \texttt{Constant}]; \texttt{SetAttributes[e, Constant}];\texttt{SetAttributes[}\Omega,\;\texttt{Constant}]\,;\;\texttt{SetAttributes}[\delta,\;\texttt{Constant}]\,
```
 \blacksquare Solution requires two expansions:

Clear[ξ , e, Fef, e00, e01, e02, e03, f00, f01, f02, f03] $\xi[\mathbf{x}_+] := \mathtt{f00}[\mathbf{x}] + \delta \mathtt{f01}[\mathbf{x}] + \delta^2 \mathtt{f02}[\mathbf{x}] + \delta^3 \mathtt{f03}[\mathbf{x}]$ e := e00 + δ e01 + δ ² e02 + δ ³ e03

 \blacksquare The differential equation is:

$$
\begin{aligned}\n\text{Fef}[\xi_{-}, \mathbf{e}_{-}, \mathbf{x}_{-}; \mathbf{x}, \delta_{-}; \delta] &:= \\
D[D[\xi, \mathbf{x}], \mathbf{x}] - \frac{2 \, m \, \Omega \, \mathbf{x}}{h} D[\xi, \mathbf{x}] + \left(\frac{2 \, m \, e}{h^2} - \frac{m \, \Omega}{h}\right) \xi - \\
\delta \left(\frac{\sqrt{2 \, m \, \mu}}{h} \mathbf{x}^2 D[\xi, \mathbf{x}] - \left(\frac{\sqrt{2 \, \mu \, m^3 \, \Omega^2}}{h^2} \mathbf{x}^3 + \frac{m^2 \, (\Omega^2 - \omega^2)}{h^2} \mathbf{x}^2 - \frac{\sqrt{2 \, m \, \mu}}{h}\mathbf{x}\right) \xi\right)\n\end{aligned}
$$

Using the expansions of ξ **and e we get:**

C1 = D[Fef[$\xi[x]$, e, x, δ], $\{\delta, 3\}$ /. $\delta \rightarrow 0$

$$
\frac{12 e03 m f00 [x]}{h^2} + \frac{12 e02 m f01 [x]}{h^2} + \frac{12 e01 m f02 [x]}{h^2} +
$$

\n
$$
6 \left(-\frac{\sqrt{2} x \sqrt{m \mu}}{h} + \frac{\sqrt{2} x^3 \sqrt{m^2 \mu \Omega^2}}{h^2} + \frac{m^2 x^2 (-\omega^2 + \Omega^2)}{h^2} \right) f02 [x] +
$$

\n
$$
6 \left(\frac{2 e00 m}{h^2} - \frac{m \Omega}{h} \right) f03 [x] - \frac{6 \sqrt{2} x^2 \sqrt{m \mu} f02' [x]}{h} -
$$

\n
$$
\frac{12 m x \Omega f03' [x]}{h} + 6 f03" [x]
$$

17

■ The term proportional to δ^1 is obtained as:

 $f00[x_] := 1;$ $e00 := hQ / 2;$ e01 := $\frac{h (\omega^2 - \Omega^2)}{4 \Omega}$ f01[x_] := $\frac{m (-\omega^2 + \Omega^2)}{4 h \Omega} x^2 + \frac{\sqrt{m} \sqrt{\mu}}{3 \sqrt{2 h}} x^3$ f02[x_] := $\frac{-3 h \mu \Omega + m^2 (\omega^2 - \Omega^2)^2}{16 h m \Omega^3} x^2 +$ $\frac{-2 \, h \, \mu \Omega + m^2 \, \left(\omega^2 - \Omega^2\right)^2}{32 \, h^2 \, \Omega^2} x^4 + \frac{m^{3/2} \, \sqrt{\mu} \, \left(-\omega^2 + \Omega^2\right)}{12 \, \sqrt{2} \, h^2 \, \Omega} x^5 + \frac{m \, \mu}{36 \, h^2} x^6;$ e02 := $\frac{h (3 h \mu \Omega - m^2 (\omega^2 - \Omega^2)^2)}{16 m^2 \Omega^3}$ $f03[x_] := a1x + a2x^2 + a3x^3 + a4x^4 + a5x^5 + a6x^6 + a7x^7 + a8x^8 + a9x^9;$ $EQ0 = C1 / x \rightarrow 0$ $EQ1 = D[CI, x]/ . x \rightarrow 0$ EQ2 = D[C1, {x, 2}]/ $x \to 0$ EQ3 = D[C1, {x, 3}]/ . $x \to 0$ EQ4 = D[C1, {x, 4}]/ . $x \to 0$ EQ5 = D[C1, {x, 5}]/ . $x \to 0$ $\mathbb{E} \mathbb{Q} \mathsf{6} = \mathbb{D} \left[\mathbb{C} \mathbb{1} \, , \ \left\{ \mathbf{x} \, , \ \mathsf{6} \right\} \right] / \quad . \ \mathbf{x} \to 0$ $\mathbb{E} \mathbb{Q} \mathbb{7} = \mathbb{D} \left[\texttt{C1}, \ \{ \mathbf{x}, \ \mathbb{7} \} \ \right] / \quad \mathbf{x} \rightarrow 0$ $\mathbb{E} \mathbb{Q} \mathsf{8} = \mathbb{D} \left[\texttt{C1}, \ \{ \mathbf{x}, \ \mathsf{8} \} \right] / \quad . \ \ \mathbf{x} \rightarrow 0$ EQ9 = D[C1, {x, 9}]/ . $x \to 0$

```
Simplify[PowerExpand[Solve]
         {EQ0 = 0, EQ1 = 0, EQ2 = 0, EQ3 = 0, EQ4 = 0, EQ5 = 0, EQ6 = 0, EQ7 = 0,}EQ8 = 0, EQ9 = 0}, {a1, a2, a3, a4, a5, a6, a7, a8, a9, e03}]]]
{{a1 -> 0, e03 -> \frac{h (\omega^2 - \Omega^2) (-6 h \mu \Omega + m^2 (\omega^2 - \Omega^2)^2)}{32 m^2 \Omega^5},<br>
a4 -> \frac{(\omega^2 - \Omega^2) (-5 h \mu \Omega + m^2 (\omega^2 - \Omega^2)^2)}{64 h^2 \Omega^4},<br>
a5 -> \frac{\sqrt{\mu} (-3 h \mu \Omega + m^2 (\omega^2 - \Omega^2)^2)}{48 \sqrt{2} h^2 \sqrt{m} \Omega^3}, a8 -> \frac{m^2 \mu (-\omega^2 + \Omega^2)}{144 h\text{a3}\rightarrow 0\text{,~a6}\rightarrow -\ \frac{\text{m }(\omega^2-\Omega^2)\,\left(\ -6\,\,\text{h }\mu\Omega+ \ \text{m}^2\,\left(\omega^2-\Omega^2\right)^2\right)}{384\,\,\text{h}^3\,\Omega^3} \text{,}a7 \rightarrow \frac{\sqrt{m} \sqrt{\mu} \left(-2 h \mu \Omega + m^2 (\omega^2 - \Omega^2)^2\right)}{96 \sqrt{2} h^3 \Omega^2}\}
```
The n=0 energy to order δ^3 is obtained summing e00+ e01+e02+e03:

Simplify[ener03]

$$
\frac{h (6 h \mu \Omega (-\omega^2 + 2 \Omega^2) + m^2 (\omega^6 - 5 \omega^4 \Omega^2 + 15 \omega^2 \Omega^4 + 5 \Omega^6)}{32 m^2 \Omega^5}
$$

 $\overline{3}$

5.1.2 Wavefunction of 1^{st} excited state to order δ^3

The *Mathematica* code to evaluate the 1^{st} excited state of the wavefunction to order $\delta^3, \ i.e. \ \psi_1^{(3)}$ $I_1^{(3)}(x)$ is $Psi0.nb,$

Expression for ψ in the first excited state up to order δ^3

SetAttributes**#**m, h, **Z**, **P**, e, **:**, **G**, Constant**'**;

21

 $\xi[x] = 2 x \sqrt{\frac{m \sqrt{-\omega^2 + \Omega^2}}{h}}$ $\delta\left(\frac{2\,\sqrt{2}\,\sqrt{h}\,\sqrt{\mu}\,\left(-\omega^2+\Omega^2\right)^{1/4}}{\text{m}\,\Omega^2}-\frac{2\,\sqrt{2}\,\,\text{x}^2\,\sqrt{\mu}\,\left(-\omega^2+\Omega^2\right)^{1/4}}{\sqrt{h}\,\Omega}\right.+\nonumber\\$ $\frac{m^{3/2} x^3 (-\omega^2 + \Omega^2)^{5/4}}{2 h^{3/2} \Omega} + \delta^2 \left(\frac{x^3 \mu (-\omega^2 + \Omega^2)^{5/4}}{2 \sqrt{h} \sqrt{m} \Omega^4} + \frac{m^{5/2} x^9 \mu (-\omega^2 + \Omega^2)^{5/4}}{160 h^{7/2} \Omega} + \right)$ $\frac{x^6 \sqrt{\mu} (-\omega^2 + \Omega^2)^{1/4} (60 h \mu \Omega - 7 m^2 (\omega^2 - \Omega^2)^2)}$ $\frac{120\sqrt{2}h^{5/2}0^3}$ $x^4 \sqrt{\mu} (-\omega^2 + \Omega^2)^{1/4} (2 h \mu \Omega - m^2 (\omega^2 - \Omega^2)^2)$ $\frac{1}{4 \sqrt{2} h^{3/2} \text{ m } \Omega^4}$ $\frac{\sqrt{\mathfrak{m}} x^{5} (-\omega^{2} + \Omega^{2})^{5/4} (7 h \mu \Omega + 2 m^{2} (\omega^{2} - \Omega^{2})^{2})}{64 h^{5/2} \Omega^{4}}$ $m^{3/2}$ x⁷ $(-\omega^2 + \Omega^2)^{5/4}$ $(-76 h \mu\Omega + 3 m^2 (\omega^2 - \Omega^2)^2)$ $\frac{1}{576 h^{7/2} \Omega^3}$ $3\sqrt{h}\sqrt{\mu}$ $(-\omega^2 + \Omega^2)^{1/4}$ $(-4h\mu\Omega + 3m^2(\omega^2 - \Omega^2)^2)$ $4\sqrt{2}$ m³ Ω⁶ $x^{2} \sqrt{\mu} \left(-\omega^{2} + \Omega^{2}\right)^{1/4} \left(27 h \mu \Omega + 7 m^{2} \left(\omega^{2} - \Omega^{2}\right)^{2}\right)$ $4\sqrt{2}\sqrt{h} m^2 \Omega^5$ $\frac{m x^8 \sqrt{\mu} \left(-\omega^2 + \Omega^2\right)^{1/4} \left(-40 h \mu \Omega + 9 m^2 \left(\omega^2 - \Omega^2\right)^2\right)}{560 \sqrt{2} h^{7/2} \Omega^2}$ $\delta^3\,\left(\frac{{\bf x}^3\,\mu\,\left(-\omega^2+{\Omega}^{\,2}\right)^{5/4}}{2\,\sqrt{\rm h}\,\sqrt{\rm m}\,\,\Omega^4}+\frac{{\rm m}^{5/2}\,{\bf x}^9\,\mu\,\left(-\omega^2+{\Omega}^{\,2}\right)^{5/4}}{160\,{\rm h}^{7/2}\,\Omega}\right.+$ $x^6 \sqrt{\mu} \left(-\omega^2 + \Omega^2\right)^{1/4} \left(60 h \mu \Omega - 7 m^2 \left(\omega^2 - \Omega^2\right)^2\right)$ $\frac{120\sqrt{2}h^{5/2}0^3}$ $x^4 \sqrt{\mu} (-\omega^2 + \Omega^2)^{1/4} (2 h \mu \Omega - m^2 (\omega^2 - \Omega^2)^2)$ $4\sqrt{2 h^{3/2} \text{ m }\Omega^4}$ $\sqrt{\mathfrak{m}} x^5 (-\omega^2 + \Omega^2)^{5/4}$ $(7 h \mu \Omega + 2 m^2 (\omega^2 - \Omega^2)^2)$ $\frac{1}{64 h^{5/2} \Omega^4}$ $\frac{m^{3/2} \mathbf{x}^7 \left(-\omega^2 + \Omega^2\right)^{5/4} \left(-76 \ln \mu \Omega + 3 m^2 \left(\omega^2 - \Omega^2\right)^2\right)}{576 \ln^{7/2} \Omega^3}$

■ The expression for ξ up to δ^3 is:

 $\overline{\mathcal{L}}$

 $Psi0.nb$

$$
\frac{3\sqrt{h}\sqrt{\mu}(-\omega^2+\Omega^2)^{1/4}(-4h\mu\Omega+3m^2(\omega^2-\Omega^2)^2)}{4\sqrt{2}m^3\Omega^6}+\frac{x^2\sqrt{\mu}(-\omega^2+\Omega^2)^{1/4}(27h\mu\Omega+7m^2(\omega^2-\Omega^2)^2)}{4\sqrt{2}\sqrt{h}m^2\Omega^5}+\frac{4\sqrt{2}\sqrt{h}m^2\Omega^5}{560\sqrt{2}h^{7/2}\Omega^2}-\frac{2}{3}\}
$$

 \blacksquare The expression for ψ is:

 $\gamma = \sqrt{\mu m/2}/3 h;$

 $\beta = m \Omega / (2 h)$;

 $h = 1$; $m = 1$; $\mu = 1$; $\Omega = 1$; $\delta = 0$; $\omega = 0$;

$$
\psi[\mathbf{x}] = \texttt{FullSimplify}\left[\texttt{Exp}\left[-\gamma(\mathbf{x}^2)\right]^{1.5} - \beta \mathbf{x}^2\right] \xi[\mathbf{x}]\right];
$$

Plot $[\psi[x], \{x, -3, 3\}]$

 δ = 1;

 $\psi[\textbf{x}] = \texttt{FullSimplify}\Big[\texttt{Exp}\big[-\gamma\ (\textbf{x}^2\big)^{1.5} -\beta\ \textbf{x}^2 \big]\ \xi[\textbf{x}]\Big] ;$

 $\overline{\mathbf{3}}$

 $Psi0.nb$

Psi0.tex

5.1.3 Wavefunction of 1^{st} excited state to order δ^5

The *Mathematica* code to evaluate the 1^{st} excited state of the wavefunction to order $\delta^5, \ i.e. \ \psi_1^{(5)}$ $I_1^{(5)}(x)$ is $Psi2.nb,$

Expression for ψ in second excited state to order δ^5

SetAttributes**#**m, h, **Z**, **P**, e, **:**, **G**, Constant**'**;

 $26\,$

The expression for ξ **to order** δ^5 **is:**

$$
\begin{split}\n\mathcal{E}[x] & = 2 + \frac{4 \pi x^2 \sqrt{-\omega^2 + \Omega^2}}{h} + \frac{2 \sqrt{2} x \sqrt{\mu} (\Omega + 9 \sqrt{-\omega^2 + \Omega^2})}{\sqrt{\pi} \Omega^2} \\
& \delta^2 \left(- \frac{\pi x^6 \mu (\Omega + 6 \sqrt{-\omega^2 + \Omega^2})}{h \Omega} + \frac{2 \sqrt{2} x \sqrt{\mu} (\Omega + 9 \sqrt{-\omega^2 + \Omega^2})}{\sqrt{\pi} \Omega^2} \right) + \frac{3 \sqrt{2} \mu^2 (\Omega + 12 \sqrt{-\omega^2 + \Omega^2})}{3 \sqrt{2} \hbar^2 \Omega^2} \\
& \frac{\pi^{3/2} x^5 \sqrt{\mu} (\omega^2 - \Omega^2) (\Omega + 6 \sqrt{-\omega^2 + \Omega^2})}{3 \sqrt{2} \hbar^2 \Omega^2} + \frac{3 x^4 \mu (3 \Omega + 26 \sqrt{-\omega^2 + \Omega^2})}{8 \hbar \Omega^2} \\
& \frac{x \sqrt{\mu} (-4 \omega^2 (2 \Omega + 3 \sqrt{-\omega^2 + \Omega^2}) + \Omega^2 (8 \Omega + 13 \sqrt{-\omega^2 + \Omega^2}))}{2 \sqrt{2} \sqrt{\pi} \Omega^4} \\
& \frac{\sqrt{\pi} x^3 \sqrt{\mu} (2 \omega^2 (13 \Omega + 6 \sqrt{-\omega^2 + \Omega^2}) - \Omega^2 (26 \Omega + 15 \sqrt{-\omega^2 + \Omega^2}))}{6 \sqrt{2} \hbar \Omega^3} \\
& \delta^3 \left(- \frac{\pi^{3/2} x^9 \mu^{3/2} (\Omega + 6 \sqrt{-\omega^2 + \Omega^2})}{28 \sqrt{2} \hbar^3 \Omega} + \frac{7 \pi^2 x^8 \mu (\omega^2 - \Omega^2) (\Omega + 6 \sqrt{-\omega^2 + \Omega^2})}{144 \hbar^3 \Omega^2} - \frac{\pi x^6 \mu (\Omega^2 (337 \Omega - 201 \sqrt{-\omega^2 + \Omega^2}) + \omega^2 (-337 \Omega + 246 \sqrt{-\omega^2 + \Omega^2}))}{576 \hbar^2 \Omega^3} + \frac{1}{\sqrt{2} \Omega^2} (\sqrt{2} \rho^2 + \Omega^2) (\rho^2 + \Omega^2 -
$$

$$
4 \omega^2 \Omega \left(551 \Omega + 175 \sqrt{-\omega^2 + \Omega^2} \right) + \Omega^3 \left(1172 \Omega + 709 \sqrt{-\omega^2 + \Omega^2} \right) \bigg) \bigg) + \frac{6 \pi^2 x^{12} \mu^2 \left(\Omega + 6 \sqrt{-\omega^2 + \Omega^2} \right)}{560 \text{ h}^4 \Omega} + \frac{67 \text{ m}^{5/2} x^{11} \mu^{3/2} \left(\omega^2 - \Omega^2 \right) \left(\Omega + 6 \sqrt{-\omega^2 + \Omega^2} \right)}{9072 \sqrt{2} \text{ h}^4 \Omega^2} + \frac{1}{360640 \text{ h}^4 \Omega^3} \left(\ln x^{10} \mu \left(-413 \text{ m}^2 \left(\omega^2 - \Omega^2 \right)^2 \left(\Omega + 6 \sqrt{-\omega^2 + \Omega^2} \right) + \frac{1}{9216 \text{ h}^2 \Omega^2} \right) + \frac{1}{9216 \text{ h}^2 \ln \Omega^5 \sqrt{-\omega^2 + \Omega^2}} \bigg) + \frac{84 \ln \mu \Omega \left(41 \Omega + 302 \sqrt{-\omega^2 + \Omega^2} \right) \bigg) + \frac{1}{9216 \text{ h}^2 \ln \Omega^5 \sqrt{-\omega^2 + \Omega^2}} \bigg) + \frac{2}{3216 \text{ h}^2 \ln \Omega^5 \sqrt{-\omega^2 + \Omega^2}} \bigg) + \frac{4 \Omega^3 \left(3212 \Omega + 2975 \sqrt{-\omega^2 + \Omega^2} \right) \bigg) + \frac{1}{4 \Omega^3 \left(3212 \Omega + 2975 \sqrt{-\omega^2 + \Omega^2} \right) \bigg) + \frac{1}{4 \Omega^3 \left(3212 \Omega + 2975 \sqrt{-\omega^2 + \Omega^2} \right) \bigg) + \frac{1}{18432 \text{ h} \, \pi^2 \Omega^6 \sqrt{-\omega^2 + \Omega^2}} \bigg) + \frac{1}{23040 \text{ h}^3 \Omega^4} \left(\kappa^8 \mu \left(534 \text{ h} \mu \Omega \left(-\Omega + 2 \sqrt{-\omega^2 + \Omega^2} \right
$$

 $\overline{\mathbf{3}}$

27

28

 $(41397660 \omega^4 - 2 \omega^2 \Omega (43239093 \Omega + 10283723 \sqrt{-\omega^2 + \Omega^2}) +$ Ω^3 (45091101 Ω + 20870801 $\sqrt{-\omega^2 + \Omega^2}$) – 2 h $\mu\Omega$ (1263892170 ω^4 - ω^2 Ω (2585050669 Ω + 488260497 $\sqrt{-\omega^2 + \Omega^2}$) + Ω^3 (1321158499 Ω + 490390527 $\sqrt{-\omega^2 + \Omega^2}$))) + $(x^{9}\sqrt{\mu})(48384 \text{ m}^{4} (\omega^{2}-\Omega^{2})^{4} (3435 \omega^{2}-\Omega (3567 \Omega + 1522 \sqrt{-\omega^{2}+\Omega^{2}})) +$ 3780 $h^2 \mu^2 \Omega^2$ (-2338466 ω^2 + Ω (2396381 Ω + 820217 $\sqrt{-\omega^2 + \Omega^2}$)) h m² $\mu\Omega$ (ω^2 - Ω^2) $(1359126150 \omega^4 + 4 \Omega^3 (276580868 \Omega - 128091611 \sqrt{-\omega^2 + \Omega^2}) +$ $ω² Ω (-2465449622 Ω+ 490769819 \sqrt{-ω² + Ω²)}))$ $(6401203200 \sqrt{2} \text{ h}^4 \sqrt{\text{m}} \Omega^6 \sqrt{-\omega^2 + \Omega^2} + (\textbf{x}^5 \sqrt{\mu}) (-11340 \text{ h}^2 \mu^2)$ Ω^2 (-2217562 ω^2 + Ω (2246063 Ω + 540777 $\sqrt{-\omega^2 + \Omega^2}$) + 448 m⁴ $(\omega^2 - \Omega^2)^3$ (9020400 ω^4 – 2 $\omega^2 \Omega$ (9887757 Ω + 3296465 $\sqrt{-\omega^2 + \Omega^2}$) + Ω^3 (10763864 Ω + 6794929 $\sqrt{-\omega^2 + \Omega^2}$) + h m² $\mu\Omega$ ($-\omega^2 + \Omega^2$) $(52677100590 \omega^4 + 2 \Omega^3 (28011121177 \Omega + 12081371879 \sqrt{-\omega^2 + \Omega^2})$ $ω² Ω (108699342944 Ω+ 24015380245 $\sqrt{-ω² +Ω²})$))/$ $(508032000\sqrt{2} h^2 m^{5/2} \Omega^8 \sqrt{-\omega^2 + \Omega^2}) +$ $(x^{7}\sqrt{\mu})(2688 \text{ m}^{4} (\omega^{2}-\Omega^{2})^{3} (1638300 \omega^{4}-2 \omega^{2} \Omega (1724104 \Omega +$ $490405\sqrt{-\omega^2+\Omega^2}$ + Ω^3 (1809908 Ω + 990463 $\sqrt{-\omega^2+\Omega^2}$) -11340 $h^2 \mu^2 \Omega^2$ (-9611974 ω^2 + Ω (9735581 Ω + 2425519 $\sqrt{-\omega^2 + \Omega^2}$)) h m² $\mu\Omega$ (ω^2 - Ω^2) $(65551950930 \omega^{4} + 2 \Omega^{3} (34469781389 \Omega + 13683601903 \sqrt{-\omega^{2} + \Omega^{2}})$ $ω² Ω (134491513708 Ω + 27230410115 \sqrt{-ω² + Ω²}))) /$ $\mathbf{1}$ $\left(7112448000\sqrt{2} \text{ h}^3 \text{ m}^{3/2} \Omega^7 \sqrt{-\omega^2 + \Omega^2} \right) + \frac{1}{67737600\sqrt{2} \text{ m}^{3/2} \Omega^{10} (-\omega^2 + \Omega^2)}$ $\left(x \sqrt{\mu}\right)$ (3780 h² μ^2 Ω² (-6 ω^2 (2556629 Ω+ 7837124 $\sqrt{-\omega^2 + \Omega^2}$) + Ω^2 (15387899 Ω + 48543801 $\sqrt{-\omega^2 + \Omega^2}$) – 224 m⁴ (ω^2 - Ω^2)³ (80 ω^4 (428461 Ω + 532545 $\sqrt{-\omega^2 + \Omega^2}$) - $4 \omega^2 \Omega^2$ (17584963 Ω + 24029088 $\sqrt{-\omega^2 + \Omega^2}$) + Ω^4 (36067697 Ω + 53659927 $\sqrt{-\omega^2 + \Omega^2}$) + h m² $\mu\Omega$ (ω^2 - Ω^2) (10 ω^4 (7627902895 Ω + 13875020556 $\sqrt{-\omega^2 + \Omega^2}$) + $2 \Omega^4$ (38768784101 Ω + 76764532903 $\sqrt{-\omega^2 + \Omega^2}$ $ω² Ω²$ (153816597152 Ω+ 292239283691 $\sqrt{-ω² +Ω²)}$)) + $\left(x^3 \sqrt{\mu} \left(11340 \ h^2 \mu^2 \Omega^2 \left(4 \omega^2 \left(2246117 \Omega + 6635437 \sqrt{-\omega^2 + \Omega^2}\right) - \right)\right)\right)$ Ω^2 (9015653 Ω + 27482907 $\sqrt{-\omega^2 + \Omega^2}$) + 112 m⁴ (ω^2 - Ω^2)³ (80 ω^4 (980087 Ω + 1065090 $\sqrt{-\omega^2 + \Omega^2}$) - $4 \omega^2 \Omega^2$ (40411631 Ω + 49597056 $\sqrt{-\omega^2 + \Omega^2}$) +

 $\overline{5}$

30

```
\Omega^4 (83253739 \Omega+ 113592974 \sqrt{-\omega^2 + \Omega^2}) –
      h m<sup>2</sup> \mu\Omega (\omega^2 -\Omega^2) (20 \omega^4 (6009428840 \Omega+ 9704399403 \sqrt{-\omega^2 + \Omega^2}) +
             2 \Omega^4 (61402004081 \Omega+ 110651866243 \sqrt{-\omega^2 + \Omega^2}) –
             ω<sup>2</sup> Ω<sup>2</sup> (242992584962 Ω+ 415301128121 \sqrt{-ω<sup>2</sup> + Ω<sup>2</sup>)})))/(203212800\sqrt{2} \ln m^{7/2} \Omega^9 (-\omega^2 + \Omega^2))
```
The expression for ψ **to order** δ^5 **is:**

 $\gamma = \sqrt{\mu m/2}/3 h$

```
\beta= m \Omega / (2 h)
```
 $h = 1$; $m = 1$; $\mu = 1$; $\Omega = 1$; $\delta = 0$; $\omega = 0$;

$$
\psi[\mathbf{x}] = \texttt{FullSimplify}\Big[\texttt{Exp}\Big[-\gamma (\mathbf{x}^2)^{1.5} - \beta \mathbf{x}^2\Big] \xi[\mathbf{x}] \Big];
$$

Plot $[\psi[x], \{x, -3, 3\}]$

- Graphics -

$$
\delta = 1;
$$
\n
$$
\psi[\mathbf{x}] = \text{FullSimplify}\left[\text{Exp}\left[-\gamma (\mathbf{x}^2)^{1.5} - \beta \mathbf{x}^2\right] \xi[\mathbf{x}]\right];
$$

 $\overline{7}$

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