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Logarithmic perturbation theory: Applications and limitations

G. Y. Ndefru and S. Duwa
Department of Physics, Bayero University, Kano, Nigeria

The time independent, non-degenerate standard perturbation theory is compared with the alternate treatment of perturbation theory called logarithmic perturbation theory (LPT). For determining the non-degenerate ground state the LPT is, in principle, easier to apply than standard perturbation theory. This is because, as opposed to the standard perturbation method which requires the knowledge of the complete set of eigenvalues and eigenfunctions of the unperturbed system, for the LPT one only needs to know the ground state wave function of the unperturbed system, the energy correction to the next lower order and some easily computable coupling constants. However, in reality, the LPT is a simpler method to apply when the ground state wavefunction is exponential in nature. But as shown here for trigonometric unperturbed wave function the LPT leads to integrals which have no analytical solutions thereby making LPT more difficult and less accurate method than the standard perturbation approach.

1.0 Introduction

In quantum mechanics there are relatively few real physical systems that can be solved exactly. Approximation methods are therefore very important in all applications of the theory. One of the most important approximations is the perturbation theory. Others methods of approximation, at least found in elementary textbooks, are the variational principle and the WKBJ approximation. What we call standard perturbation theory is the one originally derived by Schrodinger himself to for harmonic oscillation and for hydrogen atom equations [Hameka, 2004]. This approach is found in almost any elementary quantum textbook and is also known as Raleigh–Schrodinger perturbation theory. The most common perturbation cases that are usually discussed are in: the particle in a box, particle moving through a potential barrier, the harmonic oscillator, the rigid rotor and the hydrogen atom. On the order hand, LPT which was developed by Aharonov and Au [1979] are not well known and are only found in research [see e.g Au and Aharonov, 1979; Imbo and Sukhtame, 1984]. The authors usually claim that it is an easier approach to use over the conventional method. In this article, we try to show that the claim is an over generalization by showing examples where LPT is more difficult to use than the standard perturbation theory.

Someone may argue that the general availability of computers renders this effort as unnecessary, in fact, if only the numerical values of energy eigenvalues, for example, are needed, both techniques cannot compete in accuracy with the simplest programs. A counter to the above argument is that, getting the values is not always the end of the story, but sometimes, the insight one gets, even in the lowest level of approximation are beyond just numbers.

We have limited this study to non-degenerate ground state. This was because even though the LPT can also be used to calculate energy corrections to higher energy states, the treatment is similar to the ground state except that, here, care needs to be taken in removing the zero's of the wave functions before transforming to $S(x)$ (Imbo and Sukhtame, 1984).

2.0 The Standard Perturbation Theory

We use this approximation method for cases in which the Hamiltonian H describing the system can be regarded as the sum of another Hamiltonian H_0 of a closely related problem (which is exactly solvable with known

eigenvalues E_n and eigenfunctions φ_n) and energy H_1. which can be viewed as a perturbation on the system described by H_0. H can be written as:

$$H\psi = E\psi \tag{2.1}$$

where
$$H = H_0 + H_1 \tag{2.2}$$

and
$$H_0\varphi_0 = E_n^0\phi_n \tag{2.3}$$

with
$$< \phi_n \mid \phi_n > = 1 \tag{2.4}$$

It is convenient to consider the Hamiltonian H as below

$$H = H_0 + \lambda H_1, \quad 0 \le \lambda \le 1 \tag{2.5}$$

and
$$E_1 = (\phi_n, H_1\phi_n) = <n|H_1|n> 0 \tag{2.6}$$

Which is the expression for expectation value of H_1 for the unperturbed state n (Gasiorowicz, 2003). Hence the energy corrected to the first order is

$$E \approx E_0 + \lambda E_1, \ \ \lambda = 1 \tag{2.7}$$
$$\approx E_0 + <\psi_0 \mid H_1 \mid \psi_0>$$

The first order correction to wavefunction is

$$\psi_1 = \sum a_m^{(1)}\phi_m \tag{2.8}$$

where $\sum$ is the summation over the discreet eigenfunctions and

$$a_m^{(1)} = \frac{<m|H_1|n>}{E_n^0 - E_m^0} \tag{2.9}$$

The second order corrections, ψ_2 and E_2, in terms ϕ_n are (Schiff, 1968)

$$\psi_2 = \sum a_m^{(2)}\phi_m, \quad a_n^{(2)} = 0 \tag{2.10}$$

and
$$E_2 = \sum_{n \ne m} \frac{|<m|H_1|n>|^2}{E_n^0 - E_m^0} \tag{2.11}$$

giving
$$E_2 \approx E_n^0 + <n|H_1|n> + \sum_{n \ne m} \frac{|<m|H_1|n>|^2}{E_n^0 - E_m^0} \tag{2.12}$$

and

$$\psi_2 \approx \phi_n + \sum_{k \ne n} \phi_k \left[\frac{<k|H_1|n>}{(E_n^0 - E_k^{0)})} \left(1 - \frac{<n|H_1|n>}{(E_n^0 - E_k^0)} \right) + \sum_{k \ne n} \sum_{m \ne n} \frac{<k|H_1|m><m|H_1|n>}{(E_n^0 - E_m^0)(E_n^0 - E_k^0)} \right] \tag{2.13}$$

Third order perturbations are also calculated through expansions to give (Dalgarno and Lewis, 1955)

$$E_3 = \sum_k \frac{<n|H_1|k>}{(E_n^0 - E_k^0)} \left[\sum_m \frac{<k|H_1|m>}{(E_n^0 - E_m^0)} - \frac{<k|H_1|n><n|H_1|n>}{(E_n^0 - E_k^0)} \right] \tag{2.14}$$

and
$$a_k^{(3)} = \frac{a_k^{(2)}E_1 + a_k^{(1)}E_2 - \sum_m a_m^{(2)} <k|H_1|m>}{E_k^0 - E_n^0} \tag{2.15}$$

3.0 The logarithmic perturbation method

We have just looked at the standard way of doing perturbation on bound states in non-relativistic quantum mechanics. While the calculation of the first order energy correction E_1 is straight forward, the formulae for higher - order correction E_n involves summation over all possible eigenstates, which often cannot be explicitly formed even for simple perturbing potentials.

An alternative method of doing perturbation theory, which yields new expressions for any - other correction E_n to an unperturbed bound state energy, which do not involve cumbersome sums over intermediate unperturbed states has been developed by Imbo and Sukhatme (1984). In one dimension, these corrections, E_n can be evaluated using a simple explicit form containing a small number of integrals. In more than one dimension the approach is systematic

but calculations require the solution of well - defined partial differential equations. For order n = 2 this equation is identical to that of the aforementioned Dalgarno and Lewis method

This approach is called the Logarithmic Perturbation Theory (LPT) in which we first change the wave function in one - dimension to S(x) = lnψ(x), which converts the linear time independent Schrodinger wave equation into a non - linear Ricatti equation. As in the standard perturbation we will start with the time independent Schrodinger wave motion.

$$H\psi(x) = E\psi(x) \tag{3.1}$$

where, $$H \approx H_0 + \lambda H_1 \tag{3.2}$$`

$$H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx} + V_0(x) \tag{3.3}$$

and H_1 is the perturbing potential.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx} + [V_0(x) + H_1(x)]\psi(x) = E\psi(x) \tag{3.4}$$

Letting ψ(x) = exp[S(x)], that is,

$$S(x) = \ln\psi(x) \tag{3.5}$$

we see that

$$S'(x) = \frac{1}{\psi(x)}\frac{d\psi(x)}{dx} \tag{3.6}$$

$$S''(x) = \frac{1}{\psi(x)}\left[\frac{d^2\psi(x)}{dx^2} - \frac{1}{\psi(x)}\left(\frac{d\psi(x)}{dx}\right)^2\right] \tag{3.7}$$

After some substitutions and some little rearrangements we have

$$\frac{\hbar^2}{2m}\left[S''(x) + (S(x))^2\right] + V_0(x) + \lambda H_1(x) - E = 0 \tag{3.8}$$

We now expand E and $S'(x)$ in orders of λ:

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \ldots \tag{3.9}$$

$$S'(x) = C_0(x) + \lambda C_1(x) + \lambda^2 C_2(x) + \ldots \tag{3.10}$$

Substituting the above equations in equation (3.4) and grouping terms in like orders of λ will give us:-
for λ^0

$$-\frac{\hbar^2}{2m}[C_0'(x) + C_0^2(x)] + V_0(x) - E_0 = 0 \tag{3.11}$$

Therefore $$C_0'(x) + C_0^2(x) = -\frac{2m}{\hbar^2}[V_0(x) - E_0] \tag{3.12}$$

for λ^1:

$$-\frac{\hbar^2}{2m}[C_1'(x) + 2C_0(x)C_1(x)(x)] + H_1(x) - E_1 = 0 \tag{3.13}$$

Therefore $$C_1'(x) + 2C_0(x)C_1(x) = -\frac{2m}{\hbar^2}[H_1(x) - E_1] \tag{3.14}$$

and so on.
For λ^n:

$$C_n'(x) + 2C_0(x)C_n(x) = -\frac{2m}{\hbar^2}[E_n(x) - \sum_{s=1}^{n} C_s(x)C_{n-s}(x)] \tag{3.15}$$

Equations (3.14) - (3.15) are linear differential equations, which are solvable by using the method of integrating factors. Looking at equation (3.12) we can see that it is the equation for the unperturbed problem, the solution of which is the unperturbed wave function $\psi_0(x)$.
Let us now calculate the orders of corrections. For the first order we obtain

$$C_1(x)\,|\psi_0(x)|^2 = \frac{2m}{\hbar^2}[H_1(x) - E_1]\,|\psi_0(x)|^2\,dx \tag{3.16}$$

which leads to the standard first order perturbation theory result for E_1 namely,

$$E_1 = \int_{-\infty}^{\infty} H_1(x)\,|\psi_0(x)|^2\,dx = <\psi_0(x)\,|\,H_1\,|\,\psi_0(x)> \tag{3.17}$$

The second order as

$$E_2 = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} C_1^2(x)\,|\psi_0(x)|^2\,dx = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} |\psi_0(x)|^2 \left|\int_{-\infty}^{x} |\psi_0(y)|^2\,[V_1(y) - E]dy\right|^2 dx \tag{3.18}$$

Proceeding in the same manner, one can solve for C_n and E_n. The results obtained from solving equation (3.15) are

$$E_n = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\sum_{s=1}^{n-1} C_s(x)C_{n-s}(x)\right)|\psi_0(x)|^2\,dx \tag{3.19}$$

$$\frac{d}{dx}\left[C_n(x)\,|\psi_1(x)|^2\right] = -\left(\frac{2m}{\hbar^2}E_n + \sum_{s=1}^{n-1} C_s(x)C_{n-s}(x)\right)|\psi_0(x)|^2 \tag{3.20}$$

and

$$C_n(x)\,|\psi_0(x)^2| = -\int_{-\infty}^{\infty}\left(\frac{2m}{\hbar^2}E_n + \sum_{s=1}^{n-1} C_s(x)C_{n-s}(x)\right)|\psi_0(x)|^2 \tag{3.21}$$

Equations (3.19) – (3.21) are valid for $n \geq 2$.

The total energy is then written as $E = E_0 + E_1 + E_2 + \ldots$and even though the method can be generalized to three dimensions, we would, for the purpose here, treat one dimensional problems only.

3.0 Comparisons of standard and logarithmic perturbation methods

To compare these two methods we will solve some typical problems in non-relativistic quantum mechanics using both methods.

4.1 Harmonic Oscillators

If we have a harmonic perturbation such as $H_1 = bx^2/2$, the ground state energy and wave function are $E_0 = \tfrac{1}{2}\hbar\omega$ and $\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp(-\alpha x^2/2)$, respectively, where $\alpha = m\omega/\hbar$. The LPT gives the first and the second order energy corrections as $E_0^{(1)} = \frac{b}{4\alpha}$ and $E_0^{(2)} = \frac{b^2}{16m\omega^2\alpha}$, which are exactly the same results obtained using the standard perturbation technique.

4.2 Quartic Oscillator

The first and second order corrections in the ground state eigenvalue when a simple harmonic oscillator having the reduced mass μ and the force constant k is subjected to the quartic perturbation $H = ax^4$ is derived using the two theories.

Using the standard method, the eigenvalues and eigenfunctions of the unperturbed oscillator are known to be

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \text{ and } \phi_n(x) = \left(\frac{1}{2^n n!}\sqrt{\frac{\alpha}{\pi}}\right)^{1/2} e^{-\frac{\alpha x^2}{2}} H'\left(\sqrt{\alpha}x\right)$$

where n = 0, 1, 2, …; H_0 is the Hermite polynomial and $\alpha = \mu\omega/\hbar$. The first order correction to the ground state eigenvalue resulting from H_1 is $E_0^{(1)}\left\langle\phi_0(x)\,|\,ax^4\,|\,\phi_0(x)\right\rangle = \frac{3a}{4\alpha^2}$

Because the Hermite polynomial is a recurring polynomial the eigenfunction of the harmonic oscillator is also recurring. Using the recurrence relations for the Hermite polynomials (Powell and Craseman 1962, Davydov, 1969) we find that

$$E_0^{(2)} = \sum_{k\neq 0} \frac{|\langle \phi_1 | ax^4 | \phi_k \rangle|^2}{E_0^0 - E_k^0}$$

Therefore, $$E_1^{(2)} = -2.625 \frac{a^2}{\hbar\omega\alpha^4}$$

Using the LPT, we obtain:- $$E_2 = -\frac{\hbar^2}{2\mu} \int_{-\infty}^{\infty} C_1^2(x) |\phi_0(x)|^2 \, dx$$

$$C_1(x) |\phi_0(x)|^2 = \frac{2\mu}{\hbar^2} \int_{-\infty}^{\infty} \left[H_1(x) - E_0^{(1)}\right] |\phi_0(x)|^2 \, dx$$

$$E_0^{(2)} = -\frac{3a^2}{8\alpha^4\hbar\omega}$$

The standard perturbation method and the LPT give different answers for the second order ground state eigenvalues. To continue our comparison we will deviate from exponential eigenfunctions by applying both methods to the particle in a box problem

4.3 Particle in a Box: Stark Effect

Consider an electron in a potential box having a length a. When an electric field ε is turned on in the x – direction, the electron experiences a force equal to -qε and the potential function term +qεx added to it. The potential then has the form shown in figure 1.

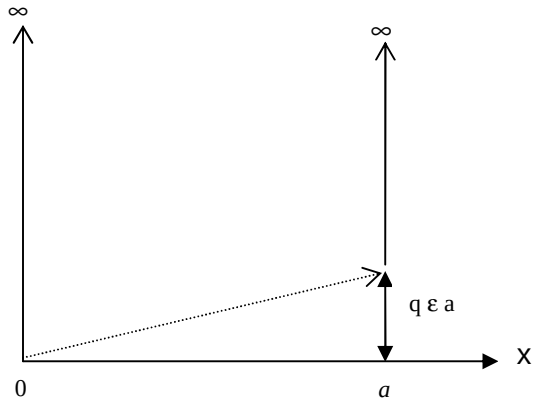

Figure 1. Infinite potential well with perturbed potential $V_1 = q \in x$.

To calculate the approximation to the ground state energy of the electron (to the first and second orders) we may assume that qεa is much smaller than the ground state energy in the absence of the electric field.

Following are obtained for first and second order energy corrections,

$$E_n^{(1)} = \frac{q \in a}{2}$$

and

$$E_1^{(2)} = -\frac{ma^4 q^2 \in^2}{\pi^2 h^2} (8.4278 + 0.01079 + 0.00035 + ...) = -8.44 \frac{ma^4 q^2 \in^2}{\pi^2 h^2}$$

Using the Logarithmic Perturbation Theory (LPT):- As already shown the, the first order energy correction is exactly the same with the expression for the Standard Method. That is,

$$E_n^{(1)} = \int_0^{\infty} H_1 |\phi_1(x)|^2 \, dx = \frac{q \in a}{2}$$

For the second order energy correction, we have

$$C_1(x)\,|\,\phi_1(x)\,|^2 = \frac{mq\in}{a\hbar^2}\left[\frac{1}{2b^2}(1-\cos 2bx)+\frac{1}{2b}\sin 2bx(a-2x)+x(x-a)\right],\quad b=\frac{\pi}{a}$$

Hence,

$$E_1^{(2)} = -\frac{mq^2\in^2}{4a\hbar^2}\int_0^{\infty}\left[\frac{1}{b^2}\sin^2 bx+\frac{1}{b^2}(a-2x)^2\cos^2 bx+\frac{x^2(x-a)^2}{\sin^2 bx}+\frac{2x(x-a)}{b^2}\right.$$
$$\left.+\frac{1}{b^2}(a-2x)\sin(2bx)+\frac{2}{b}(x^2-ax)(a-2x)\cot(bx)\right]dx$$

The third and the sixth terms in the integral above are intractable [Mangus and Oberhettinger, 1949] (at least they are insoluble using common integral tables). But reducing them using integration by parts will show that the limits will go to infinity for those terms.

It is worth noting that the same problem of non analytic integrals would arise when considering other kinds of perturbation in an infinite one dimensional box which are usually relatively easy problems under the standard perturbation theory.

4.0 Conclusions

We have compared the standard perturbation theory of quantum mechanics with the so-called Logarithmic perturbation theory (LPT). For the examples treated, in time independent non-relativistic quantum mechanics, both the standard method and the LPT worked quite well for harmonic oscillators and gave exactly the same results. We noticed that systems with exponential ground state functions were quite straight forward to calculate with LPT, even though the answer obtained in the case of a quartic perturbation differ slightly from that given by the standard perturbation approach.

The "particle-in-box" problems on the other hand are easier to solve using the standard method. Due to the fact that these systems possess trigonometric wavefunctions, LPT is incapable for energy corrections to the second and higher orders. This is because the coupling constants needed for these calculations are derived by the division of certain expressions by the square of the ground state wavefunctions.

References

[1] Au, C. K. and Aharonov, Y., "New Approach to Perturbation Theory" ,*Phys Rev Letter* 42 1582 (1979); "Logarithmic Perturbation Expansions", "*Phys. Rev. A,* 20, 2245 (1979).

[2] Dalgarno, A. and Lewis, J. T., "The Exact Calculation of Long-Range Forces between Atoms b Perturbation Theory", *Proc. Roy. Soc.* (Lond.) A233, 70 (1955).

[3] Davydov, A. S. "Quantum Mechanics" (N. E. O. Press, Maine, (1969)).

[4] Gasiorowicz, S. Quantum Physics John Wiley and Sons Inc., NJ, (2003) p 174-187.

[5] Hameka, F. H., Quantum Mechanics: A Conceptual Approach, John Wiley and Sons Inc, NJ, (2004), p108-141

[6] Imbo, T. and Suktame, U., "Logarithmic Perturbation Expansion in Non Relativistic Quantum Mechanics", *Am. J. Phys.* 52 2 140 (1984).

[7] Mangus, W. and Oberhettinger, F., "Functions of Mathematical Physics", Chelsea Publishing Co., New York (1949), p. 160.

[8] Powell, John L. and Crasemann, B., "Quantum Physics", Addison Wesley Publishing Co. Inc.,assachusetts, (1962).

[9] Schiff, L. I., "Quantum Mechanics", Mcgraw Hill Book Co., New York (1968).

[10] Schwartz, C., ,Calculations in Schrodinger Perturbation Theory", *Ann. Phys.* 6 156 (1959).

[11] Schwartz, C. and Tiamann, J. J., "Uses of Approximate Wave Functions", *Ann. Phys.* 2 170 (1959).