A SURVEY OF SOME APPROXIMATION METHODS IN MATHEMATICAL PHYSICS

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Abstract: In this paper, we examine some approximation methods often applied in mathematical physics and optimization/numerical analysis. The survey classifies the types of approximation methods particularly in quantum mechanics according to the complexity of the function involved in determining the methods. The strengths and weaknesses of these methods were considered in the various areas of application, and these information, provided users the opportunity of making appropriate choice on the usage of a particular method.

Keywords: Quantum numbers, quantum theory, ground state energy, wave function

Introduction

In literature, we observed that most quantum mechanics problems cannot be solved analytically to obtain exact solutions. Rather only few are solvable amidst making some assumptions or by the use of some mathematical models. This goes to show that approximation methods are developed and employed to solve these problems. Two primary approximation techniques are the Variational method and the Perturbation method (Ojeda-Guillien *et al*., 2016). However, there abounds other technique such as the semi-classical approximation method also known WKB method. We shall in our subsequent sections discuss the various approximation methods without bothering us with the derivation of these methods. Dashen *et al*. (1974) developed the semiclassical methods and in (1975) developed the quantum theory of solitons using the path integral approach. They applied semi-classical methods to the Sine – Gordon theory, a one – dimensional field theory characterized of having collective excitations called solitons. Stuart (2019) studied the interaction of a scalar quantum field ϕ with fixed (external) electromagnetic field $A_{\mu}^{est}dx^{\mu}$ in two dimensional space – time, in his paper "Hamiltonian quantization of solitons in ϕ_{1+1}^4 quantum field theory I, the semi-classical mass shift". Kantorovich and Krylov (2018) made landmark contributions in the literature of computational methods as domiciled in their textbook titled "Approximate Methods of Higher Analysis".

The rest of this paper will consist the following: section two will dwell on the discussions on the various approximation methods mainly in quantum mechanics; section three contains the weaknesses and strengths of these methods. Section four, dwell on some numerical problems using the methods and finally section five, the summary and conclusion.

Computational Methods in Quantum Mechanics

In this section, we shall look at four different approximation methods review their approaches to problem solving, areas of application and possible extensions.

Variational approximation method

This method also known as the Rayleigh - Ritz approximation method applies the variational principle to obtain an estimate of the ground state energy of the physical system under investigation. One essential quality of this method is domiciled in the fact that the ground state energy determined through this measure generates an upper bound for the true ground state energy. It becomes important to locate the ground state energy and the initial few states (minute quantum numbers). From some other environment, we have seen that the Schrodinger time – independent wave equation,

$$\hat{H}\psi_p = E\psi_p, \qquad (2.1)$$

Where p is the quantum number, $\hat{H}$ is a Hamilton, ψ is a wave functional, is often difficult to solve for exact solutions and so we find approximate solution through this approach. Equation (2.1) is solved for particular states; for instance, the ground state or the first initial state when we employ a trial wave function which is physically reasonable. By this, we mean, one that possesses the features of the unknown exact wave function. This wave function ψ contains a parameter ρ which is varied over a span until,

$$\left\langle \hat{H} \right\rangle = E' = \frac{\int \psi_\rho^*(x)\hat{H}\psi_\rho(x)dx}{\int \psi_\rho^*(x)\psi_\rho(x)dx} \qquad (2.2)$$

is stationary. i.e. $\dfrac{dE'}{d\rho} = 0$ (2.3)

The variational method employs the variational principle which states that the exact ground state energizes eigen value needed is the minimum value of E' or less, leads to the conclusion that

$$E_0 \approx E'(\rho_0),$$

Where $\dfrac{dE'}{d\rho} = 0$, for $\rho = \rho_0$ (2.4)

We remark here that the mean value of the Hamiltonian generated while using any trial wave function is never smaller than the exact true ground state energy of the system. However, it is exactly equal to it only if the trial wave function is equal to the ground state function. For this reason, we can say that the Rayleigh – Ritz approximation method is essential for states with low quantum numbers. It therefore serves or provides the upper bound of the ground state energy level.

Semi-classical (WKB) approximation method

The Semi-classical approximation method is due to Wentzel, Kramers and Brillouin, hence it is often also known as the WKB method. It is suitable for motions in a slowly varying potential and provides a powerful approach to examine the dynamics of quantum, field theory in particular as in the classical series of papers by Dashen – Hasslacher – Wereu and Gold – Stone – Jackin.

Through the semi – classical method, we can obtain solutions of the full non-linear interacting classical equation of motion

of various models which project as stable field configuration space time with particle properties. The idea begins with writing the wave function as in

$$\psi(x) = A(x)e^{iB(x)/h} \qquad (2.5)$$

Where *A(x)* and *B(x)* are functions must be of some specified dimensions Perisco and Enrisco (1957). Then demand that the form satisfies the time – independent Schrodinger equation. Obtain the first and second derivatives of equation (2.5). Thereafter we have;

$$[-\frac{h^2}{2m}(A''(x)+\frac{2i}{h}A'(x)B'(x)+\frac{i}{h}A(x)B''(x)+\frac{i^2}{h^2}A(x)(B'(x))^2] \qquad (2.6)$$

As $h \to 0$ in limit, this formally the same as assuming that high – order derivative of the wave function amplitude is small. By considering the different powers of *h*, in (2.6), we solve the Schrodinger equation.

This approximation approach deals with situations in which *h* is regarded as small compared to the action (energy × time or momentum × distance).

The processes employed are more or less semi- classical and are thus endeared for the cases of large quantum numbers. In order to obtain the energy levels for a bounded system, we use the result

$$A(x) = \oint \rho dx = 2\int_{x_1}^{x_2} \rho dx = \left(\frac{2n+1}{2}\right)h, n = 0,1,2 \qquad (2.7)$$

where the integral is the conventional integral over one period of the classical motion over one period of the classical motion, which is twice the integral between turning points. Using equation (2.7), we have,

$$\rho = \sqrt{2m(E-V)} \qquad (2.8)$$
$$= \rho(E,x)$$

while the turning points also rely on the unknown energy E. ρ is a function of *E* and the solution

The WKB method does not rely on integrals ie properties of the theory understudy and thus can be used both as complimentary or alternative approach to the Form Factor Perturbation approximation method for non-integral models.

Perturbation approximation method (PAM)

The whole Hamiltonian is often assumed to be divided into two sections viz $\hat{H}_0$, the main part and the $\hat{H}'$, a small section which acts as a perturbation, i.e. a small check in the system, while using the PAM. Hence,

$$\hat{H} = \hat{H}_0 + \hat{H}' \qquad (2.9)$$

In discussing perturbation theory, Heisenberg, S. and E. Schrodinger (1926), introduced time-independent perturbation after his theories in wave mechanics. The foundation of time-independent perturbation has its roots in the work of Lord Rayleigh; hence, this type of perturbation is often called Rayleigh – Schrodinger perturbation approximation.

Looking at equation (2.9) if $\hat{H}'$ is time-independent, then the theory of stationary perturbation is employed with the dominated effect of shifting the energy levels. However, if $\hat{H}'$ is time-dependent, then the time-dependent perturbation theory is applied with dominant effect causing transaction between energy levels thus can lead to scattering.

In either case, it is assumed that

(i) Everything about $\hat{H}_0$ is well known, that is both the energy eigen-states $\psi_n^{'s}$ and the energy eigen-values $E_n^{0's}$.

(ii) $\hat{H}'$ is small, thus the true energy eigen-states and the corresponding energy eigen-values are only slightly different from those of $\hat{H}_0$.

(iii) The $\psi_n^{'s}$ constitute a complete set

$$\hat{H}\,|\psi_n^{(0)}\rangle = E_n\,|\psi_n^{(0)} \qquad (2.10)$$

The essence of equation (2.10) is to obtain corrections to $E_n^{(0)}$ and ψ_n^0 which gets closer and closer to the exact eigen-state ψ_n with exact eigen-energies ψ_n. With $\hat{H}'$, a matrix of a dimension of energy, the ideas of small cannot be attached directly without comparing corresponding elements of $\hat{H}'$ some energy scale. We may introduce some quantity λ in place of $\hat{H}'$ with $\lambda\hat{H}'$ and allow $\lambda \to 0$. At the end, set $\lambda = 1$. Hence, we can solve the eigen-value equation

$$(\hat{H}_0 + \lambda\hat{H}')\psi_n\rangle = E_n\,|\psi_n\rangle \qquad (2.11)$$

By assuming the existence of expansions,

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + --- + \lambda^k E_n^{(k)} + \cdots \qquad (2.12)$$

$$\psi_n = z_n(\psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \cdots$$
$$--- + \lambda^k\psi_n^{(k)} + \cdots \qquad (2.13)$$

where the global normalization factor has to be located at the end of the calculation(this permits one to demand that the wave function correction is orthogonal to the un-perturbed state).

(I) Time – independent Perturbation Approximation Method (TIPAM)

We shall examine this method under the headings: Non-generate and the Degenerate perturbation approximation

(a) Non-degenerate TIPAM

In this case, we first assume that the energy level to be examined is not degenerate by any approximation into first order. Then, the correction to the nth energy level will be given by

$$\Delta E_n^{(1)} = \frac{\int_{-\infty}^{\infty} \psi_n^* \hat{H}'\psi_n dx}{\int_{-\infty}^{\infty} \psi_n^*\psi_n dx} \qquad (2.14)$$

$$= \int_{-\infty}^{\infty} \psi_n^* \hat{H}'\psi_n dx \qquad (2.15)$$

Given that ψ_n 's are normalized.

Using equations (2.13) and (2.15), we obtain the first order approximant by

$$E_n^{(1)} = E_n^0 + \Delta E_n^{(1)}$$
$$= E_n^0 + \left\langle \psi_n \mid \hat{H}_n \mid \psi_n \right\rangle \qquad (2.16)$$

for normalized ψ_n 's

Thereafter, the corrections to higher orders of approximation become much more complicated; however can be obtained as by definition are expected to decrease in importance. Based on this remark, we need to observe the following:

(i) The change in energy, to the first order approximation, of the nth energy level of the system, is (approximately) the expectation value of the perturbated Hamiltonian, in the nth, run perturbed state.

(ii) Suppose the above treatment is inadequate, for example, if $\left\langle n \mid \hat{H}' \mid n \right\rangle = 0$, then one has reason to go for higher orders of approximation. For instance, the correction to the energy E_n level for the second order of approximation is given by

$$\Delta E_n^{(2)} = \sum_k \frac{\left| \left\langle \psi_n \mid \hat{H}' \mid \psi_k \right\rangle \right|^2}{E_n - E_k} \qquad (2.17)$$

where is excluded from the summation. This shows clearly that the correction to the ground state energy level, to the second order approximation is always negative.

(iii) Within this class of perturbation method, only the relative phases of the components the function to states (wave functions) change with time so that the probability of locating the value E_n in a measurement of the energy is constant. With this, we state that stationary perturbation does not induce any transactions between levels. Any other observables whose corresponding operator commutes with $\hat{H}$ are also constant.

(b) Degenerate Case

Consider the expression

$$\sum_k^n \frac{\left|\langle \psi_n | \hat{H}' | \psi_k \rangle\right|^2}{E_n - E_k} \qquad (2.18)$$

and

$$\psi_n^{(k)} = -\sum_{l \neq n} \psi_l^{(k-1)} \frac{\hat{H}_{\ln}}{E_l^{(0)} - E_n^{(0)}} \qquad (2.19)$$

We know that the second order correction to energy as

$$\left\langle \psi_n^{(0)} \mid \hat{H} \mid \psi_n^{(1)} \right\rangle = E_n^{(2)} \rightarrow E_n^{(2)} = -\sum_{l \neq n} \frac{\hat{H}'_{nl} \hat{H}'}{E_l^{(0)} - E_n^{(0)}}$$

Thus, the expression for $\psi_n^{(2)}$ will be

$$\psi_n^{(2)} = \sum_{l \neq n} \psi_l^{(0)} \left(\sum_{l \neq n} \frac{\hat{H}'_{lk} \hat{H}'_{kn}}{\left(E_l^{(0)} - E_n^{(0)}\right)\left(E_k^{(0)} - E_n^{(0)}\right)} - \frac{\hat{H}'_{\ln} \hat{H}'_n}{\left(E_l^{(0)} - E_n^{(0)}\right)^2} \right) \qquad (2.20)$$

The perturbation theory fails when the denominators in expressions for $E_n^{(k)}$ and $\psi_n^{(k)}$ are either zero or comparable to the mixing matrix element. Inspite of this, there are essential situations or cases when the condition of validity of the perturbation theory is violated only for two of the lots, say N, isolated levels which do occur near degenerate. For the case, where the energy level of concern is n – fold degenerate, such that n orthonormal eigen-functions all correspond to the same energy level, however such that the stationary perturbation theory is applicable, then these n-eigen-functions are used as the basis functions in getting the $n \times n$ matrix representation of $\hat{H}'$

perturbing potential. We may thus constitute the corrections to the first order approximations of the degenerate energy level. With this, we have fully or partially removed or not removed at all; however obtain a mere shift as the eigen-values are respectively all different, partially different or all coincident.

II Time – Dependent Perturbation

Here the perturbation part of the whole Hamiltonian is time – dependent such that the presence of time – varying external forces, the time –dependent permutation theory is applied. Considering such situation, a system in an eigen-state $|k\rangle$ at time t = 0 can change character, under the influence of the external force, so that at a later time *t*, the predominant component of the wave function is in a different state $|m\rangle$. This amounts to a transition from $|k\rangle$ to $|m\rangle$.

Similarly, the expectation value of the energy of the system changes from E_k to E_m. The external force produces the work done from the difference in energy and it can be shown that the law of conservation of energy is an automatic result of the quantum treatment.

Two essential deductions can be made from the above discussion.

i) The probability amplitude for the system, initially in state $|k\rangle$, will after time *t*, and in the presence of the perturbation $\hat{H}(t)$ remain in the state $|k\rangle$ and is given by

$$S_k = \exp\left[\frac{-i}{h}\int_0^1 \hat{H}'_{kk} dt\right] \square\, 1 - \frac{i}{h}\int \hat{H}_{kk} dt \square\, 1$$

ii) The probability amplitude in the same condition above but in the presence of the perturbation $\hat{H}'(t)$ transfer into the state $|m\rangle$, is given by

$$S_m = \frac{-i}{h}\int_0^1 \hat{H}'_{kk} e^{-(E_k - E_n)\frac{t}{h}} dt \qquad (2.21)$$

so that $|C_m|^2$ is the probability of the system transferring from state $|k\rangle$ to state $|m\rangle$ after time *t*.

Under these conditions, we experience a variety of conclusion, such as constant cooperation and perturbation harmonic in time. In constant perturbation, $\hat{H}'$ is either time dependent while switched on at *t = 0* and off at time *t* or $\hat{H}'(t)$ is time independent, so that

$$S_k = \exp\left(-t\hat{H}'_{kk}\frac{t}{h}\right) \qquad (2.22)$$

which corresponds to an energy shift $\hat{H}^t_{kk}$, in agreement with first order stationary perturbation result.

Similarly, for C_m, we get

$$S_m = -\frac{1}{h}\hat{H}'_{mk}\int \exp\left[-i\left(E_k - E_m\right)\frac{t}{h}\right]dt$$

$$= -\frac{1}{h}\hat{H}'_{mk}\left.\frac{\exp\left[-i\left(E_k - E_n\right)\frac{t}{h}\right]}{-i\left(E_k - E_n\right)\frac{1}{h}}\right|_0^t$$

$$S_m = \hat{H}'_{mk}\frac{\exp\left[-i\left(E_k - E_m\right)\frac{t}{h}\right]-1}{\left(E_k - E_m\right)} \qquad (2.23)$$

Thus, the probability of locating the system in the state $|m\rangle$ after time *t* is given by

$$|S_m|^2 = \frac{|\hat{H}'_{mk}|^2}{\left(E_k - E_m\right)^2}\left|\exp\left[-i\left(E_k - E_m\right)\frac{t}{h}\right]-1\right|^2$$

Hence,

$$|S_m|^2 = \frac{|\hat{H}'_{mk}|^2}{\left(E_k - E_m\right)^2}(2)\left\{1-\cos\left(E_k - E_m\right)\frac{t}{h}\right\}$$

$$= \frac{2|\hat{H}'_{mk}|^2}{\left(E_k - E_m\right)^2}\left\{1-\cos\left(E_k - E_m\right)\frac{t}{h}\right\}$$

$$= 4|\hat{H}'_{mk}|^2\left\{\frac{\sin^2\left(E_k - E_m\right)\frac{t}{h}}{\left(E_k - E_m\right)^2 t^2/4h^2}\right\}t^2/E_m \qquad (2.24)$$

As the limit of $E_k \to E_m$, we realized that

$$|S_m|^2 = \left|\frac{\hat{H}'_{mk}}{h^2}\right|^2 t^2 \qquad (2.25)$$

We can see that the probability of transition within the non-continuous degenerate situation grows as the square of time time*t*. The above discussion dwells on individual final states in locating their transition probability per unit. However, if the final states considered together as a bundle are continuous so that they are described by a density of states, $\rho(E)$, then the transition probability per unit time, W is given by

$$W = \frac{d\rho}{dt} = \frac{2\pi}{h}\rho(E)|H'_{mk}|^2 \qquad (2.26)$$

This is the Fermi Golden Rule, applicable in situations of weak perturbations, where ρ, the transition probability is

$$\rho = \sum_{E_m > E_k}|S_m(t)|^2 = \sum_{E_m = E_k} 4|H'_{mk}|\frac{\sin^2(E_k - E_m)\,t/2h}{(E_k - E_m)}$$

where perturbation harmonic in time displays a character in which the Hamiltonian is explicitly
time – dependent and thus possesses a harmonic, time dependence. In such a situation, the perturbation, assume the form $H(x,t)$ such as

(i) $\hat{H}'(x,t) = \hat{H}(x)e^{i\psi t}$ or $\hat{H}'(x)cos\psi t$

(ii) $\hat{H}'(x,t) = \hat{H}'(x)\sin\psi t$ or $\hat{H}'(x)cos\psi t$

then for the first pair, we have

$$|S_m(t)|^2 = 4|\hat{H}'_{mk}|^2\frac{\sin^2\left[\left(\left(E_k - E_m\right)\pm h\psi\right)^{t/2h}\right]}{\left(E_k - E_m \pm h\psi\right)^2} \qquad (2.27)$$

indicating that the two scenarios lead to the transition from $|k\rangle$ state to $|m\rangle$ with appreciable probability only at $E_m = E_k \pm h\psi$. In a similar situation, with (ii) i.e. with $\hat{H}'(x)\sin\psi t$,

$$S_m(t) = -\frac{-H'_{mk}(x)}{2i}\left[\frac{\exp[i\left(E_m - (E_k - h\psi)\right)^{t/h} - 1]}{\left(E_m - (E_k - h\psi)\right)} - \frac{\exp[i\left(E_m - (E_k - h\psi)\right)^{t/h} - 1]}{\left(E_m - \left(E_k + h\psi\right)\right)}\right]$$

Or $\hat{H}'(x)\cos\psi t$:

$$S_m(t) = \frac{-1}{2h}\hat{H}_{mk}(x)\left[\frac{e^{t[E_m - (E_k - h\psi)t/h]} - 1}{\left([E_m - (E_k + h\psi)\right)} + \frac{e^{t[E_m - (E_k - h\psi)t/h]} - 1}{\left([E_m - (E_k - h\psi)\right)}\right] \qquad (2.28)$$

Weaknesses and strengths of APM

We shall discuss in this section the merits and demerits of the various methods so far surveyed in quantum mechanics.

In Perturbation Approximation Method, one of the merits of this method lies in an admixture of states with $l \neq n$ being small as long as

$$\left\| \frac{V_{lN}}{E_l^{(0)} - E_n^{(0)}} \right\| \ll 1$$

and the sum over l converges fast enough. This is a major condition which justifies the use or application of the perturbation theory. Secondly, the PAM turns a child of necessity, where the Hamiltonian can be written as an exact solvable piece plus small correction.

This method is equally saddled with some difficulties among which are:

To locate corrections to $\psi_n^{(0)}$ and $E_n^{(0)}$, which draw us closer to the exact eigen- states with exact

eigen-energies ψ_n under the assumptions that $\hat{H}$ is small. As long as $\hat{H}$ is small and with its matrix form and a dimension of energy, the notion of small cannot be attached to it directly without comparing matrix elements of $\hat{H}$ to some energy scale. Secondly, the need to know the wave-function corrections up to $\psi_n^{(k-1)}$ to find $\psi_n^{(k)}$, which is then used to determine $\psi_n^{(k)}$ persists in higher orders, making the scheme slightly increasing in complexity for large k.

It is a fact that the PAM fails when the denominator in the expressions for $E_n^{(k)}$ and $\psi_n^{(k)}$ are either zero or comparable to the mixing matrix element i.e. when

$$E_n^{(k)} \left| E_l^{(0)} - E_n^{(0)} \right| \leq \left| \hat{H}_{\ln} \right|.$$

The Variational Approximation Method (VAM) in its standard form enables us to find ground state properties in a complex system. With trial states containing hundreds and even thousands of variational parameters, the evaluation and minimization of the cost functional J is done by computers (in the multi-dimensional Hilbert space of particle coordinates, J is often simulated by Monte Carlo). The most recent tools employed here, are from quantum information science when Vrieze and Verstraete (2017) introduced matrix product and tensor network states. A glaring example, is quantum chemical calculations where people can do 200 electrons and calculate energies with relative accuracy of about 0.1%, a remarkable achievement. VAM is a powerful tool for examining the dynamics of quantum field theory in particular, as in the classical series of papers by Mashens – Hasslacher – Wereu and Goldstone – Jackson. The method empowers us to obtain solutions of the full non-linear interacting classical equation of motion of various models, which projects as stable field configuration in space – time with particle properties.

The Semi-classical Approximation Method (SAM)

The method paves way for the link between quantum mechanics and classical mechanics.

It is also an advantageous tool for locating accurate results under circumstances when the potential is relatively smooth. There is also, good physical concern for this functional form. For instance, it is a fact that a particle travels in a constant potential is described by a plane wave function De^{ipx} with $p = \sqrt{2m(E-V)}$. Thus, if this potential is smooth, i.e., does not change much on the state, then locally, the plane wave described should be also valid; however with locally defined momentum $\rho(x)$ adjusted to the current value of the potential, we observed that the only

difficulty with the replacement

$$\rho(x) \Rightarrow \int_0^x \sqrt{2m(E - \hat{H}(x))}\, dx \qquad (2.29)$$

is that, if we do something with the wave assumption then the current density $i = |c|^2 \rho(x)/m$, will thus decrease while for smooth potentials we do not expect any reflections. The Semi-classical approximation method is characterized of some matching conditions.

One of such condition, is that near the points, where $E = V(x)$ called the classical turning points, the semi-classical momentum goes to zero. This invalidates the condition

$$L(X) \geq \frac{h}{\rho(x)} = \frac{\lambda(x)}{2\pi} \qquad (2.30)$$

where L is the length scale over which the function $A(x)$ changes greatly, so as $A''(x) \ll \frac{A}{l^2}$ results. However, equation (2.30) leaves with an incomplete description, such that if we have been able to fathom how to match them in order to have a common state and obtain health to match the energy quantization condition.

Numerical Illustrations

We shall consider solving some problems applying some of the techniques discussed so far in this paper.

Problem I

(i) Determine the energy eigen values for a simple harmonic oscillator moving along the $x-axis$ with the characteristic frequency ω. Use the WKB approximation method.

(ii) Using the Rayleigh – Ritz approximation method and a suitable trial wave – function containing β^2 as parameter, given that the ground state energy of a simple harmonic oscillator was

$$E'(\beta^2) = \frac{7h^2}{6m\beta^2} + \frac{1}{24} mw^2 \beta^2$$

Find the approximate ground state energy .

The Wentzel, Kramers and Brillouin – WKB method demands that we use the result of equation (2.7), i.e.

$\oint \rho dx = 2\int_{x_0}^{x_1} \rho dx = (n + \frac{1}{2})h, n = 0,1,2,$ and for the specified simple harmonic oscillator,

$$\rho = \sqrt{2m(E - mw^2 x^2/2)}$$

and the turning points are observed to occur at $E = mw^2 x^2/2$, i.e. at x = $\pm\sqrt{2E/mw^2}$

Applying equation (8) above, we have

$$2\int_{-\sqrt{2E/mw^2}}^{\sqrt{2E/mw^2}} \sqrt{2m(E - mw^2 x^2/2)}\, dx = (n + \tfrac{1}{2})h$$

By substituting a new variable as in $x = \sqrt{2E/mw^2}\cos\theta$, then we have

$h(n + \frac{1}{2}) = \frac{4E}{w}\int_0^{\pi} \sin^2\theta d\theta = 2\pi E/w,$ and so

$$h(n + \tfrac{1}{2}) = 2\pi E/w$$

Thus,

$$E = (n + \tfrac{1}{2})hw$$

By considering a trial wave function with as the ground energy eighen values for the simple harmonic oscillator.
In our second question, we are required to find the approximate ground state energy, given that an analytical ground state energy of a simple harmonic oscillator

By considering a trial wave function with β^2 parameter, we obtain the approximate ground state energy by the Rayleigh – Ritz approximation first by observing that the expectation value of the Hamiltonian

$$\left\langle \hat{H} \right\rangle = E'(\beta^2) = \frac{7h^2}{6m\beta^2} + \frac{1}{24}mw^2\beta^2$$

$$= \frac{7h^2}{6m}\left(\beta^2\right)^{-1} + \frac{1}{24}mw^2\left(\beta^2\right).$$

At the minimum,

$$\frac{dE'(\beta^2)}{d\left(\beta^2\right)} = -\frac{7h^2}{6m\beta^4} + \frac{1}{24}mw^2 = 0$$

$$\therefore \frac{7h^2}{6m(\beta^2)^2} = \frac{1}{24}mw^2,$$

Such that, $(\beta^2)^2 = \frac{7h^2 * 24}{6m^2w^2}$ and taking square roots we have

$$\beta^2 = \sqrt{\frac{28h^2}{m^2w^2}} \Rightarrow \beta = 2\sqrt{7}\,\frac{h}{mw}$$

Hence, by substituting β_0^2 into $E'(\beta_0^2)$ we obtain the approximate ground state energy

Problem II

Consider a particle of mass m, determine the ground state energy, to the first order approximation, of a perturbed isotropic three dimensional harmonic oscillator with characteristic frequency ω, given that the perturbing potential

$\hat{H}^{\tau} = ae^{-br^2}$, and that the ground state of the oscillator is described by the wave function

$\psi_0 = \left(\frac{k}{\pi hw}\right)^{\frac{3}{4}} \exp\left(-\frac{kr^2}{2hw}\right)$, where *a*, *b* and *k* are constants.

With the system given,

$$\hat{H} = \frac{\hat{\rho}^2}{2m} + \frac{1}{2}mw^2r^2 + ae^{-br^2} = \hat{H}_0 + \hat{H}^{\tau},$$

where $\hat{H}_0 = \frac{\hat{\rho}^2}{2m} + \frac{1}{2}mw^2r^2$ and $\hat{H}^{\tau} = ae^{-br^2}$

Then, we define the ground state energy in the absence o the perturbation as

$$E_0^0 = \left(n + \frac{3}{2}\right)hw = \frac{3}{2}hw.$$

It is obvious, that is normalized. Therefore, the correction to the ground state energy, in the presence of the perturbation and to the first order approximation, is given by

$$\Delta E_0^{(1)} = \left\langle \psi_0 \left| \hat{H}^{\tau} \right| \psi_0 \right\rangle = \left(\tfrac{k}{\pi hw}\right)^{3/2} a\int \exp\left(-\left(\frac{kr^2}{2hw} + br^2\right)\right) d^3r$$

Recall that in a hemi-spherically symmetric wave function,

$$\int d^3r = 2\pi\int_0^{\infty} r^2 dr$$

In view of this,

$$\Delta E_0^{(1)} = \left(\tfrac{k}{\pi hw}\right)^{3/2} 2\pi a\int r^2 \exp\left(-r^2\left(\frac{k}{hw} + b\right)\right) dr$$

$$= \left(\tfrac{k}{\pi hw}\right)^{3/2} 2\pi a\left(\frac{1}{2}\right)\sqrt{\frac{\pi}{\left(\frac{k}{hw} + b\right)^3}}$$

$$= \left(\frac{k}{\pi hw}\right)^{\frac{3}{2}} \pi a\sqrt{\frac{h^3w^3\pi}{(k + hbw)^3}}$$

$$= \left(\frac{k}{\pi hw}\right)^{\frac{3}{2}} \pi a\left(\frac{hw\pi}{(k + hbw)}\right)^{\frac{3}{2}} = a\left(\frac{k}{(k + hbw)}\right)^{\frac{3}{2}}$$

$$\therefore E_0^1 = \sum_{j=0}^{1} \Delta^{(j)} E_0^{(j)} = \frac{3}{2}hw + a\left(\frac{k}{(k + hbw)}\right)^{\frac{3}{2}},$$

which is the ground state energy to the first order approximation.

Conclusion

We have been able to study the Variational Approximation Method, the semiclassical approximation method and the Perturbation approximation method, in which we have within the non-generate class there exists the time independent perturbation approximation method and time-dependent perturbation method, each of these exudes different characteristics. Within the generate class of the perturbation approximation methods, we noticed that the PAM fails when the denominators in expressions for $E_n^{(k)}$ and $\psi_n^{(k)}$ in equation (20) are either zero or comparable to the mixing matrix element. Despite this shortfall, the PAM is most vital approximation methods applied in quantum mechanics and in general mathematical physics. The weaknesses and strengths discussed in this paper, create an apple opportunity for end – users to make more precise choice when applying any of the discussed methods.

Conflict of Interest

The authors declare that there is no conflict of interest reported in this work.

References

Andreev VK 2015. Basic methods for solving equations of mathematical physics. *Journal of Computational Methods and Algorithms*, Vol. 1.

Dashen RF, Hasslacher B & Neveu A 1974. Nonperturbative methods and extended – hadron models in field theory.I. Semiclassical functional methods *Journal of Physics Review* D, 10: 1414.

Dashen RF, Hasslacher B & Neveu A 1975. Particle spectrum in model field theories from Semi-classical functional integral techniques. *Phys. Rev*. D, 11: 3424.

Heisenberg W & Schrodinger E 1925. The Editors of Encyclopedia Britannica Biography, Discoveries & Survey –"Chemical bonding and the quantum

mechanical model" and "Principles of Physical Science and Characteristics".

Ojeda-Guillen D, Mota RD & Granados VD 2016. A generalized Jaynes-Cummings Model: The relativistic parametric amplifier and single trapped ion. *Journal of Mathematical Physics*, 57(6).

Persico E (Translated by Tammer GM) 1957. Fundamentals of Quantum Mechanics, Prentice - Hall, Inc. Englewood Cliffs, N. J.

Stuart DM 2019. Hamiltonian quantization of solitons in ϕ^4_{1+1} Quantum Field Theory I. The Semi-classical mass shift. *Journal of Mathematical Physics*, Xiv: 1904.02588v1

Vibok A & Balint–Kurti GG 1992. Reflection and transmission of waves by a complex potential – a semi-classical Jeffreys – Wentzel – Kramers – Brillouin treatment. *Journal of Chemical Phyiscs*, 96, https://doi-org/10.1063/1.462414