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Option Pricing beyond Black-Scholes Model: Quantum Mechanics Approach

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ABSTRACT

Based on the analog between the stochastic dynamics and quantum harmonic oscillator, we propose a market force driving model to generalize the Black-Scholes model in finance market. We give new schemes of option pricing, in which we can take various unexpected market behaviors into account to modify the option pricing. As examples, we present several market forces to analyze their effects on the option pricing. These results provide us two practical applications. One is to be used as a new scheme of option pricing when we can predict some hidden market forces or behaviors emerging. The other implies the existence of some risk premium when some unexpected forces emerge.

Keywords:
Black-Scholes model
Quantum harmonic oscillator
Quantum finance

1. Introduction

The option pricing is a crucial issue in finance. The Black-Scholes (BS) model gives a guideline to price options by the risk-free scheme, which assumes the portfolio satisfies the no-arbitrage condition, perfectly hedge, invariant interests, no transaction cost and the continuous evolution of prices [1]. However, recently one discovers that above assumptions cannot hold in the practical finance markets, such as inconstant the risk-free interest rate, or non-continuously evolution, and fluctuate volatility [2], which implies that the log return distribution (return is equal to the future price minus the original price) deviates normal (Gaussian) distribution. These phenomena induce a lot of interests to modify the BS method [3-7]. Belal E. Baaquie proposed a path integral method to optimize the evaluation of path-dependent options [3]. By an elasticity variance model, Beni Lauterbach and Paul Schultz take the variant interest into account to give a new scheme of price [4]. Moreover, Louis O. Scott proved that the accurate option prices can be computed via Monte Carlo simulations when the variance changes randomly [4,5]. Interestingly, H. Kleinert and J. Korbel claimed that the prices of options can also be evaluated by the double-fractional differential equation and its solution provide a more reliable hedge comparing with BS formula [6]. Further, Lina Song and Weiguo Wang optimized the fractional BS Option pricing model by Finite Difference Method to give the solution of the difference equation [7]. More recently, Robert C. Merton generalized the stock return distribution to give an option pricing formula for the discontinuous returns [8]. Most importantly, considering the price distribution, R. N. Mantegna used Levy Walk...
instead of original random walk and he got a new price distribution deviating from normal distribution which can be applied into the BS Model \[^{[9]}\]. These studies on the generalized BS model provide many ways to improve the BS model and to make the option price close the realistic finance market. In fact, there exist some hidden market forces, such as shorting or buying an underlying asset in finance market, which drive the dynamics of finance market and make the stochastic process of the finance market deviate Gaussian distribution. This non-Gaussian effect should modify the option pricing. Therefore, in this paper, we will propose the market-force concepts to describe the stochastic dynamics of finance market based on the quantum mechanics approach. The stochastic dynamics of finance market is described by the wave function, which follows the Schrödinger equation. The hidden market forces as the market potential driving the stochastic dynamics of finance market, which make the dynamics deviate the Gaussian process and modify the BS model which give several schemes of option pricing. In Sec. II, we present the market-force model of option pricing based on quantum mechanics. In Sec. III, we propose several schemes of option pricing based on this model and discuss their advantages and financial meanings. Finally, we give the summary and conclusions in Sec. IV.

2. Market Force Model of Stochastic Dynamics

2.1 Black-Scholes Model

The dynamics of finance market is a stochastic process. The efficient market theory assumes that there does not exist the arbitrage space, which implies that the stochastic dynamics process is a Guassian process. The option pricing of the BS theory is based on the efficient market theory and the scheme of option pricing is assumed to be risk free. The European call and put options are priced by

\begin{equation}
  c = S_0 N(d_1) - Ke^{-rT} N(d_2) \quad \text{(1)}
\end{equation}

\begin{equation}
  p = Ke^{-rT} N(-d_1) - S_0 N(-d_2) \, , \quad \text{(2)}
\end{equation}

where

\begin{equation}
  N(d_1) = \frac{\ln \left( \frac{S_0}{K} \right) + (r \pm \sigma^2 / 2)T}{\sigma \sqrt{T}} \quad \text{(3)}
\end{equation}

and \( d_1 = d_2 - \sigma \sqrt{T} \). \( S_0 \) is the current price of stock or asset and their corresponding delivery (strike) price \( K \) if the option is exercised. \( r \) is the risk-free rate and \( \sigma \) is the volatility of asset. \( T \) is the time to maturity of the option. \( N(d_1) \) is the cumulative distribution function, which is expressed as

\begin{equation}
  N(d_1) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{d_1} e^{-x^2 / 2} dx \, , \quad \text{(4)}
\end{equation}

where \( N(d_2) \) is the probability for the call option exercised in a risk-free world. The expression \( S_0 N(d_1) e^{-rT} \) is the expected stock price at time \( T \) in a risk-free world when stock prices less than the strike price are counted as zero.

It can be seen that the cumulative distribution function plays a role of probability in the risk-free market. When we consider a finance market driven by some market force, shorting or buying, the Guassian probability distribution of \( N(d_1) \) can be generalized to non-Guassian probability distribution. We look for some hints from quantum mechanics how option pricing work in a non-Guassian dynamics.

2.2 Analog between Finance Market and Quantum Harmonic Oscillator

In general, the evolution of finance market is a stochastic dynamical process. The BS theory provides an option pricing scheme in a risk-free world, which implies that the dynamical process of finance market is a Guassian process. In quantum world the quantum state emerges also by a stochastic dynamics, in which the probability density is expressed in terms of the norm of wave function. The wave function evolution is driven by the Schrödinger equation. Therefore, we can find an analog between the finance market and quantum mechanics.

(1) The finance market corresponds to quantum bounded systems.

(2) The stochastic dynamics of finance market corresponds to the dynamics of quantum bounded systems.

(3) The hidden shorting or buying in finance market corresponds to the intrinsic force or potential in quantum bounded systems.

(4) The integrand function \( \frac{1}{\sqrt{2\pi}} e^{-x^2 / 2} \equiv P_{bs}(x) \) of \( N(d_1) \) corresponds to the probability density \( P(x) = |\psi|^2 \) of the quantum bounded systems. Further, the BS model corresponds to the ground state of quantum harmonic oscillator, namely, \( P_{bs}(x) = P_{bs,0}(x) \). (See the following demonstration)

(5) The cumulative distribution function of the Black-Scholes model can be written as

\begin{equation}
  N(d_1) = \int_{-\infty}^{d_1} P_{bs}(x) \, dx = \int_{-\infty}^{d_1} P_{bs,0}(x) \, dx \quad \text{(5)}
\end{equation}

This analog between finance market and quantum me-
mechanics provides a way to modify the integrand function of the BS model and give some new schemes of option pricing. Notice that this integrand function has the same form of the ground state wave function of quantum harmonic oscillator, we start from the one-dimensional quantum harmonic oscillator. The potential of the harmonic oscillator is

\[ V(x) = \frac{1}{2} \text{m} \omega^2 x^2 \]  \hspace{1cm} (6)

and the Hamiltonian of the quantum harmonic oscillator is given by\(^{[12]}\)

\[ H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} \text{m} \omega^2 x^2. \]  \hspace{1cm} (7)

The stationary Schrödinger equation is written as

\[ \frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \left( E - \frac{\text{m} \omega^2}{2} x^2 \right) \psi = 0. \]  \hspace{1cm} (8)

The wave function in the ground state can be solved\(^{[12]}\)

\[ \psi_{g,\text{HO}}(x) = \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\alpha^2 x^2/2}, \]  \hspace{1cm} (9)

where \( \alpha = \sqrt{\frac{\text{m} \omega}{\hbar}} \). For convenience we set \( \alpha = \frac{1}{\sqrt{2} x_0} \), where \( x_0 = 1 \) for the dimensional consistency with \( x \), we may redefine the variable \( x = x / x_0 \) to a dimensionless variable such that the probability density in the ground state

\[ P_{g,\text{HO}}(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} = P_{\text{BS}}(x). \]  \hspace{1cm} (10)

Therefore, the ground state of quantum harmonic oscillator corresponds to the BS model. This correspondence between finance market and quantum harmonic oscillator provides a way to generalize the Black-Scholes model based on quantum mechanics approach. When we add some forces to generalize the quantum harmonic oscillator, the wave function in the ground state and its corresponding probability density deviates the Guassian form. This infers that some market forces emergence makes the finance market deviate the Guassian process and modify the BS option pricing.

The finance market force is defined by

\[ F = -\frac{dV(x)}{dx}, \]  \hspace{1cm} (11)

where \( V(x) \) is the potential of the bounded system. General speaking, force describes any local or individual behavior making finance market deviate the equilibrium state, while potential describes the global effect induced from these local or individual behaviors. Thus, the finance market force describes the behaviors of shorting or buying the underlying asset or any economic news and psychological behaviors in finance market. \( F = -\frac{dV(x)}{dx} > 0 \) means any market force pushing the asset or stock price high. \( F = -\frac{dV(x)}{dx} < 0 \) means any market resistance bringing down the asset or stock price.

It should be pointed out that the finance market forces we introduce from quantum mechanics will modify the option pricing from two ways. One is to modify \( P_{g,\text{HO}}(x) \), which means to modify \( P_{\text{BS}}(x) \) and the cumulative distribution function, the other is to modify the volatility \( \sigma \) because the force drives the probability distribution deviating from the Guassian distribution. The effective volatility can be obtained by

\[ \sigma_{\text{eff}} = \sigma \sigma_{\text{QM}}, \]  \hspace{1cm} (12)

where \( \sigma_{\text{QM}} = \sqrt{\langle x^2 \rangle_{\text{QM}} - \langle x \rangle_{\text{QM}}^2} \) and \( \langle f(x) \rangle_{\text{QM}} = \int f(x) P_{\text{QM}} \, dx \) with \( P_{\text{QM}}(x) \) being the probability density from quantum mechanics. The volatility \( \sigma_{\text{QM}} \) in the Black-Scholes formula (1) is 1 for the standard Guassian distribution.

In principle, we can design different forces to study or describe different market behaviors and modify the option pricing. When the force vanishes \( F = 1 \), the quantum system reduces to the harmonic oscillator and our model reduces to the Black-Scholes Model. Thus, the standard harmonic oscillator potential \( \frac{1}{2} \text{m} \omega^2 x^2 \) can be regarded as the natural boundary condition of finance market.

Based on this analog between the finance market and quantum harmonic oscillator, we can take different forces into account for the harmonic oscillator to generalize the BS option pricing for understanding their financial meaning.

3. Market Forces and Option Pricing

3.1 Constant Forces

Let us consider the market force be a constant \( F = -k \). It corresponds to the potential

\[ F = -k \]

where \( V(x) \) is the potential of the bounded system. General speaking, force describes any local or individual behavior making finance market deviate the equilibrium state, while potential describes the global effect induced from these local or individual behaviors. Thus, the market force describes the behaviors of shorting or buying the underlying asset or any economic news and psychological behaviors in finance market. \( F = -\frac{dV(x)}{dx} > 0 \) means any market force pushing the asset or stock price high. \( F = -\frac{dV(x)}{dx} < 0 \) means any market resistance bringing down the asset or stock price.
\[ V_x(x) = kx, \]  

where \( 0 < k \ll 1 \) is a small parameter describing the strength of the potential. Thus, the Schrödinger equation of the harmonic oscillator system with a linear potential can be written as

\[
\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \left( E - \frac{m\omega^2}{2} x^2 + kx \right) \psi = 0. \tag{14}
\]

By solving the Schrödinger equation, we obtain the solution of the wave function in the ground state

\[
\psi_g(x) = \left( \frac{1}{\sqrt{2\pi}} \right)^{1/2} e^{-\left( x - x_k \right)^2 / 4}, \tag{15}
\]

where \( x_k = \frac{k}{m\omega^2} \). The probability density defined by

\[
P_x(x) = |\psi|^2 \tag{16}
\]

where \( x \) and \( x_k \) should be viewed as dimensionless variables. Using the corresponding relation in Eqs. (5) and (10) the probability density in (16) is viewed as the integrand function of a generalized BS model, namely \( P_x(x) \approx P_{BS}(x) \). The peak of the probability density is shifted to \( x_k \), which is shown in Figure 1(a). We plot numerically the call option price versus the shift \( x_k \) in Figure 1(b).

It can be seen from Figure 1(a) that the shape of the probability density does not change and it moves to the left for the constant market force \( F < 0 \). Similarly, it will move to the right for \( F > 0 \). From the financial point of views, \( F < 0 \) means that there exists shorting the asset in finance market and \( F > 0 \), means buying behaviors in finance market. The option prices are shown in Figure 1(b), in which the dashed line is the option price for \( F = 0 \) (the BS model) and the solid line for the constant force case \( F < 0 \). When the force increases with \( k \) the call option price should decrease monotonically with \( k \) for \( F < 0 \). It matches the market behavior that sorting the underlying asset will reduce its call option price. Similarly, it should increase with \( k \) for \( F > 0 \).

3.2 Linear Forces

When we consider the market force being proportional to \( x \), \( F = -2\lambda x \), which induces the potential in finance market

\[ V_x(x) = -\lambda x^2, \]  

where \( 0 < \lambda \ll 1 \). The Schrödinger equation of the harmonic oscillator system with a quadratic potential can be written as

\[
\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \left( E - \frac{m\omega^2}{2} x^2 - \lambda x^2 \right) \psi = 0. \tag{18}
\]

Note that two potential terms are quadratic, by the standard quantum mechanical approach, \cite{12} we introduce a
where \( k \) is the elastic constant of the harmonic oscillator model. The wave function in the ground state can be obtained by

\[
\psi_g(x) = \left(\frac{\alpha_x}{\sqrt{2\pi}}\right)^{1/2} e^{-\alpha_x x^2/2}. \quad (19)
\]

where we keep \( \alpha_x x \) is a dimensionless variable. Approximately, we have \( \alpha_x \approx \alpha(1 + \frac{\lambda}{2k}) \). Thus, the probability density is given by

\[
P_x(x) &= \frac{\alpha_x}{\sqrt{2\pi}} e^{-\alpha_x x^2/2} \approx \alpha_x e^{-\frac{x^2}{2}} p_{g0}(x), \quad (19)
\]

where \( x \) returns to a dimensionless variable with neglecting \( x_0 \). It can be seen that the linear force modifies the probability density, namely generalizing the integrand function of the BS model.

Figure 2 (a) shows the comparison of the probability densities (the integrand function) between the standard BS model and the generalized harmonic oscillator with the linear force as a generalized BS model. It can be seen that the force modifies the peak height and the volatility of the probability density such that the option prices vary with the force strength seen in Figure 2 (b).

### 3.3 \( x^3 \) Forces

For the market force \( F = -3\beta x^3 \), which induces the potential in finance market

\[
V_\beta(x) = \beta x^3. \quad (20)
\]

For small \( \beta \), we use the perturbation method to obtain approximately the wave function in the ground state of the system (see Appendix A). The Hamiltonian of the system can be written as

\[
\hat{H} = \hat{H}_0 + V_\beta(x). \quad (20)
\]

where \( \hat{H}_0 \) is the Hamiltonian of the harmonic oscillator in (7). We can give the first-order approximation solution of the wave function in the ground state by the perturbative method (see Appendix C)

\[
\psi_\beta(x) = C_\beta e^{-x^4/4} \left[ 1 - \eta_\beta \left( 2x + \frac{1}{3} x^3 \right) \right], \quad (21)
\]

where \( C_\beta = \left( 1 + \frac{29}{3} \eta_\beta \right)^{1/2} \) is the normalized constant.

It can be seen that the integrand function of the BS model is generalized to (22) based on the \( x^3 \)-dependent force model. We plot the probability density versus \( \beta \) in Figure 3(a) and the corresponding call option price in Figure 3(b).

We can see from Figure 3(a) that the main peak moves to right. As \( \beta \) increase a sub-peak appears. This phenomenon can be interpreted by the collective effect in finance market in the natural boundary condition. Figure 3(b) shows the option price with \( \beta \). As \( \beta \) increases the option price goes down with shorting force, which matches our expectation.

## 3.4 \( x^3 \) Forces

Further we can consider the market force \( F = -4\gamma x^3 \), which induces the potential in finance market

\[
\]
\[ V_f(x) = \gamma x^4. \quad (23) \]

The Hamiltonian for this case can be written as
\[ \hat{H} = \hat{H}_0 + V_f(x). \quad (24) \]

Similarly, for small \( \gamma \), by the perturbative method we can obtain the first-order approximate solution of the wave function in the ground state. The solution of wave function in the first-order approximation can be given by (see Appendix C)
\[ \psi_{\xi\gamma}(x) = C_{\gamma} \left[ 1 + \frac{39}{2 \xi_{\gamma}^2} \right]^{-1/2} \left( \frac{9}{4} \left( \frac{x}{x_0} \right)^2 - \frac{1}{4} \left( \frac{x}{x_0} \right)^4 \right), \quad (24) \]

where \( C_{\gamma} = \left( 1 + \frac{39}{2 \xi_{\gamma}^2} \right)^{-1/2} \) is the normalized constant.

\( \xi_{\gamma} = \frac{\gamma x_0^4}{\hbar \omega} \) and \( 0 < \xi_{\gamma} < 1 \) can be viewed as a dimensionless small parameter. Similarly, \( x \) in (24) is a dimensionless variable with neglecting \( x_0 \). By the same way, the probability density is obtained by
\[ P_{\xi\gamma}(x) = P_{\xi\gamma}(x)C_{\gamma} \left[ 1 + \frac{39}{2 \xi_{\gamma}^2} \right]^{-1/2} \left( \frac{9}{4} \left( \frac{x}{x_0} \right)^2 - \frac{1}{4} \left( \frac{x}{x_0} \right)^4 \right)^2, \quad (25) \]

Thus, we obtain the integrand function of the BS model generalized from the \( x^3 \)-dependent force model.

In Figure 4(a), we plot the probability density versus \( \gamma \) and the corresponding call option price shown in Figure 4(b). It should be noticed that the finance market depends on both \( \gamma \) and \( x \) shown in Figure 4(a). For \( \gamma > 0 \), \( F = 0 \) means that the force is resistant for \( x > 0 \) and the force is active for \( x < 0 \). For \( \gamma < 0 \), \( F > 0 \) means that the force is active for \( x < 0 \) and the force is resistant for \( x > 0 \). As \( |\lambda| \) increases, the original price could be unstable and there exist two symmetric attractors, which push price either up or down. Figure 4(b) shows the call option price versus \( \gamma \). The call option price shows a minimum at \( \gamma = 0 \) and a maximum at \( \gamma \approx -0.14 \). When the price distribution becomes less homogeneous, the call option price will be lower. This perfectly matches the realistic situation that the less fluctuate price of underlying assets leads to a lower call option price. Furthermore, we can also apply this method to solve any other polynomial boundary conditions. For an arbitrary condition, we can expand the function with Taylor series and we can analyze the change of the call option price to an arbitrary hidden market force.

\[ V_f(x) = \gamma x^4. \quad (23) \]

3.5 Quantum Well

In finance market, if a company does not want its Underlying Asset price lower than \( S \), it is equivalent to exist a boundary condition that makes the dealing of its asset stop. From the quantum mechanics point of view, we may set up a quantum well model to simulate this behavior. The potential of quantum well is
\[ V_{\text{QW}}(x) = \begin{cases} \infty & \text{for } |x| > a \\ 0 & \text{for } |x| < a \end{cases}, \quad (27) \]

where \( a \propto \Delta S \). It implies when \( x \leq X_a \) (\( X_a \propto S - S_0 \)) the finance market is in the normal state and the market will stop if some unexpected forces make the Underlying Asset price going beyond the lower or upper bound, namely lower than \( S_0 - \Delta S \) or higher than \( S_0 + \Delta S \). \( |a| \) can be regarded as a boundary of finance market. The solution of wave function in ground state is obtained
\[ \psi_{\text{QW}}(x) = \frac{1}{\sqrt{a}} \sin \left[ \frac{\pi}{2a} (x + a) \right], \quad x \in [-a, +a], \quad (27) \]

The probability density is expressed
\[ P_{\text{QW}}(x) = \begin{cases} \frac{1}{a} \sin^2 \left[ \frac{\pi}{2a} (x + a) \right], & x \in [-a, +a] \\ 0, & x \in (-\infty, -a) \cup (a, \infty) \end{cases}, \quad (28) \]

Since the boundary of the well prevents neither the underlying price increasing too very high nor decreasing too very low, the whole distribution will be squeezed within \(-a < x < a\). The probability of the future underlying price still near current price significantly increases, but when
$x \to \pm a$, the probability decreased below the normal distribution seen in Figure 5(a). By plugging the distribution function in Eq. (29), we can plot the $c$ versus $\lambda$ curve for the call option price with $a$. The figure 5(b) shows that when $a < 0.3$, the original price does not change. The call option price is equal to $S_0 - Ke^{-rT}$. As $a$ increases the call option price will also increase. This result shows that as the price distribution becomes more homogeneous, the call option will be more expensive, which matches the realistic situation.

As illustrative examples here we present the call option pricing based on this framework. Similarly, we can also give the modification of the put option pricing in the practical application.

4. Conclusion

The BS model gives a scheme of option pricing based on the risk-free, efficient market hypothesis and the standard Gaussian stochastic dynamics of finance market. In the realistic finance market there exist various unpredictable factors, such as abnormal shorting or buying some assets, some rules or policy changes, some unexpected news and some psychological features of investors, which could break the efficient market hypothesis making the stochastic dynamics deviate from the standard Gaussian stochastic dynamics of finance market. How do we take these factors into account to generalize the Black-Scholes model for the option pricing becomes a practical problem. We discover the analog between the Gaussian stochastic dynamics and the probability density of the ground state of quantum harmonic oscillator. We propose a market force model to simulate various unpredictable market behaviors to modifying the Guassian dynamics based on quantum mechanics approach. Based on this model we give a new scheme of option pricing for various unpredictable market behaviors. The option pricing based on quantum mechanics provides a more systematic and explicit way to generalize the Guassian probability distribution for the BS model than other approaches [9].

As examples, we present several market forces to generalize the BS model and turn out their corresponding option pricing. In principle, we can generalize further this method to more complicated forces driving the finance market because any form of forces or potentials as a function of $x$ can be expanded by Taylor series. By the perturbation method we can calculate arbitrary-order approximation of wave function based on the quantum mechanics approach. On the other hand, we can also generalize the one-dimensional oscillator to the multi-dimensional oscillators, which covers various market forces and their interactions which could modify the option pricing. This study on the option pricing provides two practical hints. One is that as a new scheme of option pricing we can modify the pure BS model-based option pricing when we can predict some unexpected force emergence. The other is that when one cannot predict these unexpected forces appearing. The prediction of the option pricing based on this scheme provides some risk premium.

5. Appendix

5.1 The Quantum Harmonic Oscillator

The Hamiltonian of the quantum harmonic oscillator is given by

$$\hat{H}_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2. \quad (29)$$

The eigen wave function can be obtained by the standard quantum mechanical approach, [12]

$$\psi_n(x) = \left( \frac{\alpha}{\sqrt{\pi 2^n n!}} \right)^{1/2} e^{-\frac{\alpha^2 x^2}{2}} H_n(\alpha x), \quad (30)$$

where $\alpha = \sqrt{\frac{m \omega}{\hbar}}$. $H_n(\alpha x)$ is the Hermit polynormal function. The corresponding eigen energies are

$$E_n = \hbar \omega \left( n + \frac{1}{2} \right), \quad (31)$$

where $n = 0, 1, 2, \ldots$. DOI: https://doi.org/10.30564/jesr.v3i4.2311
5.2 The Perturbative Method

The eigen energies by the non-degenerate perturbation method are given by

\[ E_n = E_n^{(0)} + H_n^{(1)} + \sum_{m \neq n} \frac{|H_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} + \cdots, \quad (32) \]

and their corresponding wave functions are obtained by

\[ \psi_n = \psi_n^{(0)} + \sum_{m \neq n} \frac{H_{nm}}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)} + \cdots, \quad (33) \]

where \( H_{nm} = \langle \psi_n | H | \psi_m \rangle \) is the matrix element of the perturbative Hamiltonian.

5.3 The Perturbative Wave Function in the Ground State of Harmonic Oscillator

The wave function in the ground state of the harmonic oscillator can be given by

\[ \psi_g(x) = \alpha^{1/2} e^{-\alpha x^2/2}. \quad (34) \]

For convenience, we introduce the annihilation and creation operators in the Fock space, respectively \[\hat{a} = \frac{\alpha}{\sqrt{2}} \left( x + \frac{i}{\alpha} \hat{p}_x \right) \quad \text{and} \quad \hat{a}^\dagger = \frac{\alpha}{\sqrt{2}} \left( x - \frac{i}{\alpha} \hat{p}_x \right). \quad (35) \]

The occupation number representation of the position and momentum operators are given by

\[ x = \frac{\hat{a}^\dagger + \hat{a}}{\sqrt{2}\alpha}, \quad \hat{p}_x = \frac{\hat{a}^\dagger - \hat{a}}{i\sqrt{2}\alpha}. \quad (36) \]

Note that the commutative relations of the creation and annihilation operators are \([\hat{a}, \hat{a}^\dagger] = 1\) and \([\hat{a}, \hat{a}^\dagger] = [\hat{a}^\dagger, \hat{a}] = 0\), they apply on the occupation-number states and satisfy the following equations \[\hat{a} | n \rangle = \sqrt{n+1} | n+1 \rangle, \quad (40)\]

where the occupation-number states satisfy the orthonormal relation \( \langle n | m \rangle = \delta_{nm} \).

\textbf{Case 1:} \( x^2 \) forces

The perturbation Hamiltonian is given by

\[ \hat{H} = \beta x^3 = \frac{\beta}{2\sqrt{2}\alpha} \left( \hat{a} + \hat{a}^\dagger \right)^3. \quad (42) \]

The perturbation matrix elements in the ground state are expressed as

\[ H_{0m} = \langle 0 | \hat{H}^\dagger | m \rangle = \frac{\beta}{2\sqrt{2}\alpha} \langle 0 | \left( \hat{a} + \hat{a}^\dagger \right)^3 | m \rangle. \quad (43) \]

Note that \( \langle 0 | \left( \hat{a} + \hat{a}^\dagger \right)^3 | m \rangle = 3 \langle 0 | m - 1 \rangle + \sqrt{6} \langle 0 | m - 3 \rangle \), by using formula in Eq. (32), the wave function in the ground state can be given by

\[ \psi_{\beta}(x) = \psi_{\beta}^{(0)}(x) - \eta_{\beta} \left[ 3 \psi_{\beta}^{(0)}(x) + \sqrt{6} \eta_{\beta} \psi_{\beta}^{(0)}(x) \right], \quad (44) \]

where \( \eta_{\beta} = \frac{\beta x^3}{\hbar \omega} \). Note that the Hermite polynomial functions are \( H_1(x) = 2x \), and \( H_3(x) = 8x^2 - 12x \), the wave function can be expressed as

\[ \psi_{\beta}(x) = C_{\beta} e^{-x^2/4} \left[ 1 - \eta_{\beta} \left( 2x + \frac{1}{3} x^3 \right) \right], \quad (45) \]

where \( C_{\beta} = \left( 1 + \frac{29}{3} \eta_{\beta}^2 \right)^{-1/2} \) is the normalized constant.

\textbf{Case 2:} \( x^3 \) forces

The perturbation Hamiltonian is given by

\[ \hat{H} = \gamma x^4 = \frac{\gamma}{4\alpha^4} \left( \hat{a} + \hat{a}^\dagger \right)^4. \quad (46) \]

and the perturbation matrix element in the ground state is expressed as

\[ H_{0m} = \langle 0 | \hat{H}^\dagger | m \rangle = \frac{\gamma}{4\alpha^4} \langle 0 | \left( \hat{a} + \hat{a}^\dagger \right)^4 | m \rangle. \quad (47) \]

Similarly, we have \( \langle 0 | \left( \hat{a} + \hat{a}^\dagger \right)^4 | m \rangle = 3 \langle 0 | 0 \rangle + 6 \sqrt{2} \langle 0 | m - 2 \rangle + 2 \sqrt{6} \langle 0 | m - 4 \rangle \).
Similarly, by using formula in Eq. (32), the wave function in the ground state can be given by

$$\psi_r(x) = \psi_0^{(0)}(x) - \xi_r \left( 3\psi_2^{(0)}(x) + \frac{\sqrt{3}}{2} \psi_4^{(0)}(x) \right),$$  \hspace{1cm} (48)$$

where \( \xi_r = \frac{\gamma x_0^4}{\hbar \omega} \). Note that the Hermit polynomial functions are \( H_2(x) = 4x^2 - 2 \), and \( H_4(x) = 16x^4 - 48x^2 + 12 \), the wave function can be expressed as

$$\psi_r(x) = \frac{C_r e^{-x^2/4}}{(2\pi)^{1/4}} \left[ 1 + \xi_r \left( \frac{9}{4} \left( \frac{x}{x_0} \right)^2 - 1 \left( \frac{x}{x_0} \right)^4 \right) \right],$$  \hspace{1cm} (49)$$

where \( C_r = \left( 1 + \frac{39}{2} \xi_r^2 \right)^{-1/2} \) is the normalized constant.

References