The Effect of Discontinuous Wave Functions on Optimizations of VMC Calculations of Quantum Systems

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Abstract

Here, a relatively good comparison has been done between the performance results of discontinuous and continuous forms of wave function on quantum systems as well. In this project, we’ve estimated the energy of ground and first state as the expectation value of Hamiltonian of harmonic oscillator and binding energy of nucleons confined in a Yukawa potential by making use of following three wave function: exponential, linear and Gaussian form which are convenient to optimize and may be evaluated rapidly are devised and tested and we stress the advantages of using expressions which are Gaussian in the variable parameters. Exponential function is quite different from a Gaussian ones as it has a cusp at x=0, hence a discontinuity in its derivatives. We then have performed to test inaccuracy of the discontinuous wave function and energy's error of its exact value because using of exponential and linear function by mathematical statements of calculation of delta and Heaviside function and either VMC calculation of wave function optimization, as both of them will have the same result of error value. The result of our study is very promising for future applications of quantum Monte Carlo methods especially in many body systems.

Keywords: VMC calculation, Delta and Heaviside function, Discontinuity, Wave function

1. Introduction

The variational Monte Carlo (VMC) ,(DMC) [1] methods is stochastic approaches for evaluating quantum mechanical expectation values with many body Hamilton-
ians and wave functions [2]. VMC is a simple and elegant method. The VMC method is conceptually very simple. The energy is calculated as the expectation value of the Hamiltonian with an approximate many-body trial wave function [3,4]. The time independent Schrödinger equation reads

$$\hat{H} \Psi_n = E_n \Psi_n$$  \hspace{1cm} (1)

Monte Carlo methods have played an important role in our understanding of a variety of quantum systems, especially few- and many-body quantum systems with strong interactions that are difficult to treat otherwise (see, e.g., Refs. [5,6,7,8,9]). It is also well-known, however, that most quantum Monte Carlo methods [6] are formulated in such a way that they are strictly applicable only to the ground state of a quantum system, a restriction that has severely limited their applicability.

We will now proceed to see how we make use of these methods to get an estimate of the ground state energy of a quantum mechanical many-particle system, using the QVMC method. We start out with seeing how the actual energy calculation is done, then discuss how the sampling is done[6]. We then set up the actual algorithm. At the end we will discuss what is called importance sampling in the QVMC scheme. This is a way to improve upon the basic algorithm. The variational theorem of quantum mechanics states that, for a proper trial wave function $\Psi_T$, the variational energy,

$$E_v = \frac{\int \Psi_T^*(R) \hat{H} \Psi_T(R) dR}{\int \Psi_T^2(R) dR}$$  \hspace{1cm} (2)

is an upper bound on the exact ground state energy $E_0$, i.e., $E_v \geq E_0$.

To facilitate the stochastic evaluation, $E_v$ is written as

$$E_v = \int p(R) E_L(R) dR$$  \hspace{1cm} (3)

where the probability distribution $p$ is

$$p(R) = \frac{\Psi_T^2(R)}{\int \Psi_T^2(R) dR}$$  \hspace{1cm} (4)

and the local energy,

$$E_L(R) = \Psi_T^{-1} \hat{H} \Psi_T$$  \hspace{1cm} (5)

2. Monte Carlo sampling a trial wavefunction

The key problem is how to create and sample the distribution $\Psi_T^2(R)$ (from now on, for simplicity, we consider only real trial wave functions). This is readily
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done in a number of ways, possibly familiar from statistical mechanics. Probably the most common method is simple Metropolis sampling [10]. Specifically, this involves generating a Markov chain of steps by “box sampling” \( R' = R + \tilde{\zeta} \Delta \), with \( \Delta \) the box size, and \( \tilde{\zeta} \) a \( 3M \)-dimensional vector of uniformly distributed random numbers \( \zeta \in [-1,1] \). This is followed by the classic Metropolis accept/reject step, in which \( (\Psi'_f(R')/\Psi_f(R))^2 \) is compared to a uniformly distributed random number between zero and unity. The new coordinate \( R' \) is accepted only if this ratio of trial wave functions squared exceeds the random number. Otherwise the new coordinate remains at \( R \). This completes one step of the Markov chain (or random walk). Under very general conditions, such a Markov chain results in an asymptotic equilibrium distribution proportional to \( \Psi_f^2(R) \). Once established, the properties of interest can be “measured” at each point \( R \) in the Markov chain (which we refer to as a configuration). The exact wave function is a solution to the Schrodinger equation. For any but the simplest systems the form of the wave function is unknown. However, it can be approximated in a number of ways. Generally this can be done systematically through series expansions of some sort, such as basis set expansions or perturbation theory.

3. Mathematical statement of discontinuous functions

This wave function, whose shape is displayed in figure 1, is quite different from a Gaussian: it has a cusp at x=0, hence its first derivative is discontinuous at x=0. The normalization constant A can be calculated at once:

\[
\langle \Psi_0 | \Psi_0 \rangle = A^2 \int_{-\infty}^{0} e^{2\alpha x} dx + A^2 \int_{0}^{\infty} e^{-2\alpha x} dx = 2A^2 \int_{0}^{\infty} e^{-2\alpha x} dx = \frac{A^2}{\alpha^2}
\]

To find \( E_0(\alpha) \) we need to calculate the potential and the kinetic term. We can easily calculate the potential term:

\[
\langle \Psi_0 | V(x) | \Psi_0 \rangle = \frac{1}{2} m \omega^2 A^2 \int_{-\infty}^{\infty} x^2 e^{-2\alpha |x|} dx = m \omega^2 A^2 \int_{0}^{\infty} x^2 e^{-2\alpha x} dx \frac{m \omega^2}{4\alpha^2}
\]

But the kinetic energy term: is quite tricky to calculate. Since the first derivative of \( \Psi_0(x) \) is discontinuous at x=0, a careless, straightforward calculation of, which makes use of \( \langle (20) \rangle \), leads to a negative kinetic energy.
\[ \left\langle \Psi_0 \left| \frac{d^2}{dx^2} \right| \Psi_0 \right\rangle = -\left( \frac{\hbar^2}{2m} \right) A^2 \int_{-\infty}^{+\infty} e^{-\alpha x} \left\{ \frac{d^2 e^{-\alpha x}}{dx^2} \right\} dx = -\left( \frac{\hbar^2}{m} \right) A^2 \int_0^{+\infty} e^{-\alpha x} \left\{ \frac{d^2 e^{-\alpha x}}{dx^2} \right\} dx \]

\[ = \frac{\hbar^2}{m} A^2 \int_0^{+\infty} e^{-\alpha x} \left\{ \frac{d^2 e^{-\alpha x}}{dx^2} \right\} dx = -\frac{\hbar^2}{2m} \alpha^2 \]

So when the first derivative of the wave function is discontinuous, the correct way to calculate the kinetic energy term is by using (20):

\[ -\left( \frac{\hbar^2}{2m} \right) \left\langle \Psi_0 \left| \frac{d^2}{dx^2} \right| \Psi_0 \right\rangle = \]

\[ \left( \frac{\hbar^2}{2m} \right) A^2 \int_{-\infty}^{+\infty} e^{-\alpha x} \left[ \frac{d e^{-\alpha x}}{dx} \right]^2 dx = \frac{\hbar^2 A^2}{2m} \int_{-\infty}^{+\infty} e^{-\alpha x} dx = \frac{\hbar^2 A^2}{2m} \]

(9)

Because \[ A^2 \int_{-\infty}^{+\infty} e^{-\alpha x} dx = 1 \]

Why do expression”(8)” and”(9)” yield different results? The reason is that the correct expression \[ \frac{d^2 e^{-\alpha x}}{dx^2} \] must involve a delta function Figure (1). That is, the correct from of \[ d \Psi(x) \] is given by:

\[ \frac{d \Psi_0(x)}{dx} = A \frac{d e^{-\alpha x}}{dx} = -\alpha \Psi_0(x) \frac{d x}{dx} = -\alpha \Psi_0(x) \]

\[ \begin{cases} -1, x < 0 \\ 1, x > 0 \end{cases} \]

(10)

Or

\[ \frac{d \Psi_0(x)}{dx} = -\alpha [\Theta(x) - \Theta(-x)] \Psi_0(x) \]

(11)

where \[ \Theta(x) \] is the Heaviside function[11] \[ \Theta(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0 \end{cases} \].

The second derivative of \[ \psi_0(x) \] therefore contain a delta function [12]:

\[ \frac{d^2 \Psi_0(x)}{dx^2} = \frac{d}{dx} \left\{ -\alpha [\Theta(x) - \Theta(-x)] \Psi_0(x) \right\} \]

(12)

And since [13]

\[ \frac{d \Theta(x)}{dx} = \delta(x), \quad \left[ \Theta(x) - \Theta(-x) \right]^2 = 1, \delta(x) = \delta(-x) \]

Therefore we have:
\[
\frac{d^2 \Psi_0(x)}{dx^2} = -\alpha^2 [\Theta(x) - \Theta(-x)]^2 \Psi_0(x) - \alpha [\delta(x) + \delta(-x)] \Psi_0(x) = \alpha^2 \Psi_0(x) - 2\alpha \Psi_0(x) \delta(x)
\]

(13)

So the substitution of "(13)" into "(8)" leads to the same (correct) expression as "(9)"

\[
E_0(\alpha) = \frac{\hbar^2}{2m} \alpha^2 + \frac{m \omega^2}{2\alpha_0^2},
\]

(15)

The minimization of \(E_0(\alpha)\):

\[
0 = \frac{\delta E_0(\alpha)}{\delta \alpha} = \frac{\hbar^2}{m} \alpha_0 - \frac{m \omega^2}{2\alpha_0^2},
\]

(16)

Leads to \(\alpha_0^2 = \frac{m \omega}{\sqrt{2\hbar}}\) which, when inserted into"(15)", leads to:

\[
E_0(\alpha_0) = \frac{\hbar^2}{2m} \frac{m \omega}{\sqrt{2\hbar}} + \frac{m \omega^2}{\sqrt{2}} \frac{\sqrt{2}}{4} \frac{\hbar}{m \omega} = \frac{\hbar \omega}{\sqrt{2}} = 0.707 \hbar \omega
\]

(17)

This inaccurate result was expected; it is due to the cusp at \(x=0\). Now we can show that the normalization constant \(A = \left(\frac{4\alpha^3}{\pi^2}\right)^{1/2}\).

Unlike \(A e^{-|\Psi|}\), the first derivative of the trial \(\frac{A}{1+x^2}\) is continuous, hence we can use "(20)" to calculate the kinetic energy term. The ground state energy is given by:

\[
E_0(\alpha) = \langle \Psi_0(\alpha) | \hat{H} | \Psi_0(\alpha) \rangle = A^2 \int_{-\infty}^{\infty} \frac{1}{x^2 + \alpha^2} (-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m \omega^2}{x^2} \frac{1}{x^2 + \alpha}) \frac{1}{x^2 + \alpha} dx
\]

\[
- \frac{A^2 \hbar^2}{2m} \int_{-\infty}^{\infty} \frac{6x^2 - 2\alpha}{(x^2 + \alpha)^3} dx + \frac{1}{2} m \omega^2 A^2 \int_{-\infty}^{\infty} \frac{x^2}{(x^2 + \alpha)^2} dx = \frac{\hbar^2}{4m \alpha} + \frac{1}{2} m \omega^2 \alpha.
\]

(18)
The minimization of \( E_o(\alpha) \) respect to \( \alpha \) (i.e., \( \frac{\delta E(\alpha)}{\delta \alpha} = 0 \)) yields \( \alpha_0 = \frac{\hbar}{\sqrt{2m\omega}} \) which, when inserted into "(18)\), leads to

\[
E_o(\alpha_0) = \frac{\hbar\omega}{\sqrt{2}} \quad (19)
\]

This energy, which is larger than the exact value \( \frac{\hbar\omega}{2} \) by a factor \( \sqrt{2} \), is similar to that of previous part; this is a pure coincidence. The size of this error is due to the fact that the trial function \( \frac{A}{x^2 + \alpha} \) is not a good approximation to the exact wave function, which has a Gaussian form.

In those problems where the first derivative of the wave function is discontinuous at a given value of \( x \), one has to be careful when using the expression:

\[
-\langle \psi | \frac{\hbar^2}{2m} \frac{d^2}{dx^2} | \psi \rangle = -\frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} \psi^*(x) \frac{d^2\psi(x)}{dx^2} dx \quad (20)
\]

A straightforward, careless use of this expression sometimes leads to a negative kinetic energy term. One might instead consider using the following form:

\[
-\langle \psi | \frac{\hbar^2}{2m} \frac{d^2}{dx^2} | \psi \rangle = -\frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} \left| \frac{d\psi(x)}{dx} \right|^2 dx \quad (21)
\]

Node that and are identical; an integration by parts lead to:

\[
\int_{-\infty}^{+\infty} \left| \frac{d\psi(x)}{dx} \right|^2 dx = \psi^*(x) \frac{d^2\psi(x)}{dx^2} \bigg|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \frac{d^2\psi(x)}{dx^2} \frac{d^2\psi(x)}{dx^2} dx = -\int_{-\infty}^{+\infty} \frac{d^2\psi(x)}{dx^2} dx \quad (22)
\]

Since \( \psi^*(x) \frac{d\psi(x)}{dx} \) goes to zero as \( x \to \pm \infty \) (this is the case whenever \( \psi(x) \) is a bound state, but not so when \( \psi(x) \) is a plane wave). What about the calculation of \( \langle \psi | (-\hbar^2/(2m))\Delta | \psi \rangle \) in three dimensions? We might consider generalizing. For this we need simply to invoke Gauss theorem to show that:

\[
\int (\nabla \psi^*(r)).(\nabla \psi(r))d^3r = \int \psi^*(r)\Delta \psi(r)d^3r \quad (23)
\]

To see this, an integration by parts leads to the following relation:

\[
\int \psi^*(r)\nabla \psi(r)d\vec{A} = \int (\nabla \psi^*(r)).(\nabla \psi(r))d^3r \quad (24)
\]

And since, as \( S \to \infty \), the surface integral \( \int \psi^*(r)\nabla \psi(r) . d\vec{S} \) vanishes if \( \psi(r) \) is a bound state, we recover. So the kinetic energy term is given in three dimensions by:

\[
-\langle \psi | \frac{\hbar^2}{2m} \Delta | \psi \rangle = \frac{\hbar^2}{2m} \int (\nabla \psi^*(r)).(\nabla \psi(r))d^3r \quad (25)
\]
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Figure 1: Shapes of \( \Psi_0(x) = A e^{-\alpha x^2} \), \( \frac{d\Psi_0(x)}{dx} \), and \( \frac{d^2\Psi_0(x)}{dx^2} \)

3.2 Sample: calculation of discontinuous function of one-dimensional harmonic oscillator

The trial function we choose for the ground state has to be even and smooth everywhere, it must vanish as \( x \to \pm \infty \), and it must have no nodes. A Gaussian function satisfies these requirements. But what are not sure about is its width. To account for this, we include in the trial function an adjustable scale parameter \( \alpha \):

\[
\Psi_0(x, \alpha) = A e^{-\alpha x^2}
\]

(26)

A is a normalization constant. Using:

\[
\int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \frac{(2n-1)!}{(2\alpha)^n}
\]

(27)

We can show that \( A \) is given by \( A = \left( \frac{2\alpha}{\pi} \right)^{1/2} \). The expression for \( E_0(\alpha) \) is thus given by:

\[
\psi_0 \mid H \mid \psi_0 \rangle = A^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) e^{-\alpha x^2} dx
\]

\[
= A^2 \frac{\hbar^2 \alpha}{m} \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx + A^2 \left( \frac{1}{2} m \omega^2 - \frac{2 \hbar^2 \alpha^2}{m} \right) \int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx
\]

\[
= \frac{\hbar^2 \alpha}{m} \left( 1 + \frac{1}{4\alpha} \left( \frac{1}{2} m \omega^2 - \frac{2 \hbar^2 \alpha^2}{m} \right) \right) = \frac{\hbar^2 \alpha}{2m} + \frac{m \omega^2}{8\alpha}
\]

(28)

Or

\[
E_0(\alpha) = \frac{\hbar^2}{2m} + \frac{m \omega^2}{8\alpha}.
\]

(29)

The value of \( \alpha_0 \) corresponding to the lowest point of the curve, can be obtained from the minimization of \( E(\alpha) \) with respect to \( \alpha \),
Yields $\alpha_0 = \frac{m\omega}{2\hbar}$ which, when inserted into "(22)" and "(20)", leads to:

$$E_0(\alpha_0) = \frac{h\omega}{2}, \quad \Psi_0(x, \alpha_0) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{m\omega}{2\hbar}}$$

(31)

The ground state energy and wave function obtained by the variational method are identical with their exact counterparts. Let us now find the approximate energy $E_1$ for the first excited state. The trial function $\psi_1(x, \alpha)$ we need to select must be odd, it must vanish as $x \to \pm \infty$, it must have only one node, and it must be orthogonal to $\psi_0(x, \alpha_0)$ of Eq (26). A candidate that satisfies these requirements is:

$$\psi_1(x, \alpha) \propto B e^{-x^2}$$

(32)

B is the normalization constant. We can show that $B = (32\alpha^3 / \pi)^{1/4}$. Note that $\langle \psi_0 | \psi_1 \rangle$ is zero. Since the symmetric integration of an odd function is zero: $\psi_0(x)$ is even and $\psi_1(x)$ is odd. Proceeding as we did for $E_0(\alpha)$, and since $\psi_1(x, \alpha)$ is normalized, we can show that the minimization of $E_0(\alpha)$ with respect to $\alpha$ (i.e., $\frac{\partial E_1}{\partial \alpha} = 0$) lead to $\alpha = \frac{m\omega}{2\hbar}$. Hence the energy and the state of the first excited state are given by:

$$\psi_1(x, \alpha_0) = \left(\frac{4m^2\omega^2}{\pi\hbar^2}\right)^{1/4} x e^{-\frac{m\omega}{2\hbar}}$$

(33)

$$E_1(\alpha_0) = \frac{3h\omega}{2}$$

They are in full agreement with the exact expressions. The trial function

$$\psi_2(x, \alpha, \beta) = C (\beta x^2 - 1) e^{-x^2}$$

(34)

Which includes two adjustable parameters $\alpha$ and $\beta$, satisfies all the properties of the second excited state: even under parity, vanishes as $x \to \pm \infty$, and has two nodes. The term $(\beta x^2 - 1)$ ensures that $\psi_2(x, \alpha, \beta)$ has two nodes $x = \pm 1/\sqrt{\beta}$; and the normalization constant C is given by:

$$C = \left(\frac{2\alpha}{\pi}\right)^{1/4} \left[\frac{3\beta^2}{16\alpha^2} - \frac{\beta}{2\alpha} + 1\right]^{1/2}$$

(35)
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The trial function \( \psi_2(x, \alpha, \beta) \) must be orthogonal to both \( \psi_0(x) \) and \( \psi_1(x) \).

First, notice that it is indeed orthogonal to \( \psi_1(x) \), since \( \psi_2(x, \alpha, \beta) \) is even while \( \psi_1(x) \) is odd:

\[
\langle \psi_1 | \psi_2 \rangle = C \left( \frac{4m \omega}{\pi \hbar^3} \right)^{1/4} \int_{-\infty}^{\infty} x (\beta x^2 - 1) e^{-\alpha x^2} e^{-m \alpha x^2/2h} \, dx = 0
\]

(36)

As for the orthogonally condition of \( \psi_2(x) \) with \( \psi_0(x) \), it can be written as

\[
\langle \psi_0 | \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_0(x) \psi_2(x) \, dx = \left( \frac{m \omega}{\pi h} \right)^{1/4} C \int_{-\infty}^{\infty} \beta k^2 - e^{m h \omega^2 x^2} \, dx = 0
\]

(37)

This leads to a useful condition between \( \beta \) and \( \alpha \):

\[
\beta = \frac{m \omega}{h} + 2\alpha
\]

Now let us focus on determining the energy \( E_2(\alpha, \beta) \):

\[
E_2(\alpha, \beta) = C^2 \int_{-\infty}^{\infty} (\beta x^2 - 1) e^{-\alpha x^2} \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right] (\beta x^2 - 1) e^{-\alpha x^2} \, dx
\]

(38)

After lengthy but straightforward calculation, we obtain:

\[
-\frac{\hbar^2}{2m} \left( \langle \psi_2 | \frac{d^2}{dx^2} \rangle | \psi_2 \rangle \right) = \frac{\hbar^2}{2m} \left( \alpha + \frac{\beta}{2} + \frac{7\beta^2}{16\alpha} \right) C^2 \sqrt{\frac{\pi}{2\alpha}}
\]

(39)

\[
\frac{1}{2} m \omega^2 \left( \langle \psi_2 | x^2 \rangle | \psi_2 \rangle \right) = m \omega^2 \left( \frac{15\beta^2}{128\alpha^3} - \frac{3\beta}{16\alpha} + \frac{1}{8\alpha} \right) C^2 \sqrt{\frac{\pi}{2\alpha}}
\]

(40)

Hence

\[
E_2(\alpha, \beta) = C^2 \sqrt{\frac{\pi}{2\alpha}} \left( \frac{\hbar^2 \alpha}{2m} + \frac{\hbar^2 \beta}{4m} + \frac{7\hbar^2 \beta^2}{32m\alpha} + \frac{15m \beta^2 \omega^2}{128\alpha^3} - \frac{3m \beta \omega^2}{16\alpha^2} + \frac{m \omega^2}{8\alpha} \right)
\]

(41)

To extract the approximate value of \( E_2 \), we need to minimize \( E_2(\alpha, \beta) \) with respect to \( \alpha \) and to \( \beta : \hat{\alpha} E_2(\alpha, \beta) / \hat{\alpha} \alpha = 0 \) and \( \hat{\beta} E_2(\alpha, \beta) / \hat{\beta} \beta = 0 \). The two expressions we obtain will enable us to extract (by solving a system of two linear equations with two unknowns) the value of \( \alpha_0 \) and \( \beta_0 \) that minimize \( E_2(\alpha, \beta) \). This method is lengthy and quite cumbersome; \( \alpha_0 \) and \( \beta_0 \) have to satisfy the condition. We can, however, exploit this condition to come up with a much shorter
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approach: it consists of replacing the value of $\beta$ as displayed in into the energy relation, thereby yielding an expression that depends on a single parameter $\alpha$:

$$E_2(\alpha) = \left(\frac{15\hbar^2\alpha}{m} + \frac{9\hbar \omega}{8} + \frac{7m\omega^2}{16\alpha} + \frac{15m^2\omega^4}{128\hbar^2\alpha^3} + \frac{9m^2\omega^4}{32\hbar\alpha^2}\right)\left(\frac{3m^2\omega^2}{16\hbar^2\alpha^2} + \frac{m\omega}{4\hbar\alpha} + \frac{3}{4}\right)^{-1}$$

(42)

In deriving this relation we have substituted into the expression for $C$ as given by, which in turn is inserted into. In this way, we need to minimize $E_2$ with respect to one parameter only $\alpha$. This yields $\alpha_0 = m\omega / (2\hbar)$ which, when inserted into, leads to $\beta_0 = 2m\omega / \hbar$. Thus, the energy and wave function are given by:

$$E_2(\alpha_0, \beta_0) = \frac{5}{2}\hbar\omega, \quad \psi_2(x, \alpha_0, \beta_0) = \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(\frac{2m\omega}{\hbar}x^2 - \frac{m\omega}{2\hbar}\right)$$

(43)

These are identical with the exact expressions for the energy and the wave function. In Figure 2, we calculate the ground state energy of harmonic oscillator using VMC simulation. As has been seen in Figure 2, we obtain:

$$E_0(\alpha) = 0.500075 \ (h = \omega = 1) \text{ (GS)}$$

Whereas the result based on mathematical statements is: $E_0(\alpha) = \frac{\hbar\omega}{2}$

In Figure 3, we calculate the first state energy of harmonic oscillator using VMC simulation. As can be seen in Figure 2, we have obtained: $E_0(\alpha) = 1.19058 \ (h = \omega = 1) \text{ (FS)}$.

While the results based on mathematical statements for first state is:

$$E_0(\alpha) = \frac{3\hbar\omega}{2}.$$ 

Second state energy of harmonic oscillator using VMC simulation Figure 4.

$$E_0(\alpha) = 2.47652 \ (h = \omega = 1) \text{ (SS)}.$$ 

So the results based on mathematical sentences for second state is: $E_0(\alpha) = \frac{5\hbar\omega}{2}$.

In Figure 5, we plot the variations of ground state energy a system using discontinuous exponential function and then obtain the optimum energy: $E_0(\alpha_0) = 0.707111 \ (h = \omega = 1)$. While calculation based on the mathematical results of discontinuous exponential function show that $E_0(\alpha_0) = \frac{\hbar\omega}{\sqrt{2}} = 0.707\hbar\omega$

In Figure 6, we show the variation of ground state energy a system using linear function and prepare its optimum energy: $E_0(\alpha_0) = \frac{\hbar\omega}{\sqrt{2}} = 0.707117\hbar\omega$. 
Calculation based on the mathematical results of linear function, Suggest that
\[ E_0(\alpha_0) = \frac{\hbar \omega}{\sqrt{2}} = 0.707 \hbar \omega \] (accordance with Eq. (17)) that is similar to exponential function ones. In Figure 7, we plot the Binding energy of nucleons confined in the Yukawa potential using VMC calculation as well too.

Figure 2: The variation of the ground, first and second state energy a system using linear, Gaussian function and prepare the optimum energy using VMC simulation. In Figure 2-a: we calculate the ground state energy of harmonic oscillator, Figure 2-b: we calculate the first state energy of harmonic oscillator, Figure 2-c: Second state energy of harmonic oscillator (using Gaussian function). Figure 2-d: ground state energy a system using discontinuous exponential function, Figure 2-e: ground state energy a system using linear function. In Figure 2-f: we plot the Binding energy of nucleons confined in the Yukawa potential using VMC calculation.
4. Conclusion:

We hope to have convinced the reader that the VMC approach to obtaining quantum expectation values of interest in both chemical and physical problems is a very powerful one. We believe that it, in combination with fully quantum Monte Carlo procedures, will be the preferred choice in the near future, for many of the calculations performed these days by more traditional non-stochastic means. VMC is the first, and a necessary step, toward a complete quantum simulation of a system. It has the very desirable feature (often a rare one) that it can be learned, implemented, and tested in a short period of time. In this here we construct different kinds of trial wave function for VMC simulation:

1- Discontinuous exponential function.
2- Linear function.
3- Gaussian function.

In this here we construct calculation of energy different states of harmonic oscillator using discontinuous exponential function by simulation VMC. Then they calculated them by mathematical tools of the variational method all referred to similar results in VMC calculation supporting use of Gaussian form functions in these calculations.

References


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