# การใช้วิธีมอนติคาร์โลแปรผันแก้ปัญหาบ่อศักย์คู่สมมาตร

# Variation Monte Carlo Treatment of Symmetric Double-Well Potential Problem

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## บทคัดย่อ

ได้ใช้วิธีมอนติคาร์โลแปรผัน แก้ปัญหาบ่อศักย์คู่สมมาตร $V(x) = -kx^2 + \lambda x^4$ บนครึ่งโดเมนโดยพิจารณาที่ $k$ และ $\lambda$ หลายๆ ค่า ได้ค่าของพลังงานสถานะพื้นที่ได้ในหน่วยคำนวณสอดคล้องกับค่าที่ได้จากวิธีฮิลล์เด็ทท์ซึ่งเป็นวิธีที่แม่นยำสูงมาก สำหรับศักย์ชนิดนี้ ได้ขยายกราฟของฟังก์ชันคลื่นออกไปจนเต็มโดเมน และพบว่าลักษณะของความหนาแน่นของความน่าจะเป็นนั้นเป็นไปตามหลักการของการทะลุผ่านกำแพงศักย์และความสมมาตรของฟังก์ชันคลื่น

**คำสำคัญ :** วีเอ็มซี บ่อศักย์คู่กำลังสี่ ครึ่งโดเมน รูปแบบผลต่างไฟไนต์

## Abstract

We apply variation Monte Carlo method within half-domain to the symmetric double-well problem in the form $V(x) = -kx^2 + \lambda x^4$ for several values of positive $k$ and $\lambda$. The values of ground-state energy are in good agreement with the Hill determinant method, a very accurate approach for this kind of potential. In addition, the graphs of wave function are extended to full domain and are displayed We also find this method yields the probability densities that comply with tunneling principle and symmetry of wave function.

**Keywords :** VMC, quartic double-well, half domain, random values, finite-difference form.

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## Introduction

The double-well potential acts as a good model of some physical devices whose potential can be imagined as two wells at both sides with a barrier in the middle. This kind of problem has so far attracted physicists worldwide (Arias & Buenda, 1990; Balsa *et al*., 1983; Banerjee, 1978; Bansal *et al.*, 1991; Bishop & Flynn, 1988; Brickmann & Zimmermann, 1969; Fernandez *et al.*, 1985; Handy, 1992; Hodgson *et al.*, 1989; Schiffrer, 1985; Somorjai & Hornig, 1962; Witwit, 1996; Witwit & Killingbeck, 1993).

In most articles the symmetric quartic one, *i.e.* $V(x) = -kx^2 + \lambda x^4$ has been chosen to investigate, for the sake of simplicity. This symmetric potential graph has two minima with a potential barrier between two potential wells. If the particle has total energy less than the height of central barrier, one may view it as being influenced by two wells. If it initially stays in one particular well, it may eventually leak to another one by tunneling. The width and height of the central barrier depends on the parameters $k$ and $\lambda$. According to elementary Calculus, barrier height = $k^2/(4\lambda)$ and the barrier width = $\sqrt{2k/\lambda}$. Once the ratio $k/\lambda$ is large the barrier height will be high, then tunneling becomes ineffective. It follows that the wave function will decay considerably towards the origin so that the ground-state probability might resemble the first excited-state one. This reflects the truth that both ground and first-excited-state energy levels lie close to each other in this case. Otherwise, if the central well is short or narrow tunneling towards origin will be more likely, then the probability will indeed differ from the first excited state one, resulting in remarkable spacing of energy spectrum.

Several means have been applied to solve this problem, *e.g*. Hill determinant method (Witwit, 1996), analytical transfer matrix method (Zhou *et al.*, 2003), finite element method (Chaiharn, 2008), numerical shooting method (Wan-ek, 2008), phase integral method (Fröman *et al*., 1980)], gradient method (Schiffrer, 1985), coupled cluster method (Bishop & Flynn,1988) *etc*.

## Materials and Methods

In the Variation Monte Carlo method (VMC) we first assign a trial wave function, $\varphi(x)$, usually in a simple form, *e.g*. a constant throughout the domain. Then, for a given potential $V(x)$, calculate the expectation value of energy pertaining to this wave function. Of course, this energy is not a correct one yet as long as the trial wave function is still not correct either. The next step, we numerically pick up x by random and vary $\varphi(x)$ at that point by an infinitesimal amount, *i.e*. $\pm\Delta\varphi$. The sign should be plus or minus depending on which one yields lower expectation value of energy. Then continue choosing $x$ again byrandom and repeat the foregoing procedure. Randomizing $x$ up to $10^4$ times or more will spread $x$ overall domain and tend to stabilize the energy expectation value. Actually this gives us the lowest energy as desired. The procedure not only yields the ground-state energy but also the very accurate ground-state wave function in position space.

## The Hamiltonian in half-domain VMC approach

By substituting the symmetric double-well potential

$$V(x) = -kx^2 + \lambda x^4, \tag{1}$$

which we shall use throughout this article, into the energy expectation value equation, we get

$$\langle H \rangle = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_{-\infty}^{\infty} \psi^* \left( -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - kx^2 + \lambda x^4 \right) \psi \, dx}{\int_{-\infty}^{\infty} \psi^* \psi \, dx} \tag{2}$$

Being a bound-state problem, the domain can be made finite for computing purpose, *i.e*.

$$\langle H \rangle = \frac{\int_{x_{\min}}^{x_{\max}} \psi^* \left( -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - kx^2 + \lambda x^4 \right) \psi \, dx}{\int_{x_{\min}}^{x_{\max}} \psi^* \psi \, dx}. \tag{3}$$

Also, for abound-state problem the wave function can be set real, that is

$$\langle H\rangle = \frac{\int_{x_{\min}}^{x_{\max}} \psi\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - kx^2 + \lambda x^4\right)\psi\, dx}{\int_{x_{\min}}^{x_{\max}} \psi^2\, dx}. \quad (4)$$

Since all functions in the integrand are even, we may work in half domain yielding

$$\langle H\rangle = \frac{\int_{0}^{x_{\max}} \psi\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - kx^2 + \lambda x^4\right)\psi\, dx}{\int_{0}^{x_{\max}} \psi^2\, dx}. \quad (5)$$

Throughout this article, we use such computational units that $\hbar = 1$, $m = 1/2$ . This simplifies (5) to

$$\langle H\rangle = \frac{-\int_{0}^{x_{\max}} \psi\psi''\, dx + \int_{0}^{x_{\max}} \left(\lambda x^4 - kx^2\right)\psi^2\, dx}{\int_{0}^{x_{\max}} \psi^2\, dx}. \quad (6)$$

Applying by-part integration, (6) is transformed to the following one:

$$\langle H\rangle = \frac{-\int_{0}^{x_{\max}} \psi\, d\psi' + \int_{0}^{x_{\max}} \left(\lambda x^4 - kx^2\right)\psi^2\, dx}{\int_{0}^{x_{\max}} \psi^2\, dx}. \quad (7)$$

Next, we approximate the integrals with the aid of Trapezoidal rule, obtaining

$$\langle H\rangle = \frac{\sum_{i=1}^{n}\left(\frac{-2\psi_i\left(\psi_{i+1} - 2\psi_i + \psi_{i-1}\right)}{\left(\Delta x\right)^2} + \lambda\left(x_i^4\psi_i^2 + x_{i+1}^4\psi_{i+1}^2\right) - k\left(x_i^2\psi_i^2 + x_{i+1}^2\psi_{i+1}^2\right)\right)}{\sum_{i=1}^{n}\left(\psi_i^2 + \psi_{i+1}^2\right)}, \quad (8)$$

where we have divided the domain into $n$ equally small parts, each of width $\Delta x$, practically taken to be optimally small as 0.2.

Eq. (8) will be used extensively by computer program to evaluate the expectation value of energy, until we get the minimal value as stated in the previous section.

The flow chart representing algorithm in brief of this work is presented in the next page.

## Results and Discussion

We have calculated ground-state energies of this system in several cases and then compare the results with those from Hill determinant approach (Witwit, 1996), the results are shown below.

*Ground-state energies*

The following tables display numerical results of energy eigenvalues for particular value of $\lambda$ and $k$. The energies are in the computational units that $\hbar = 1$ and $\mathrm{m} = \frac{1}{2}$ . For the parameters, we have used $\Delta x = 0.1$, $\Delta\psi = 0.02$ since, as long as we tried, they give satisfactory results whereas smaller values would cause much longer computing time with similar outcomes. In the same way, we have used $\psi(x) = 0.5$ almost throughout the domain for the initial unnormalized wave function, for the sake of simplicity as shown in Fig.1 below. The figure also displays the final wave function after The percent difference is calculated with respect to those obtained from Hill Determinant method which is regarded as an approach that yields very accurate results (Hautot, 1986; Hautot & Magnus, 1979; Hautot & Nicolas, 1983; Znojil, 1982).

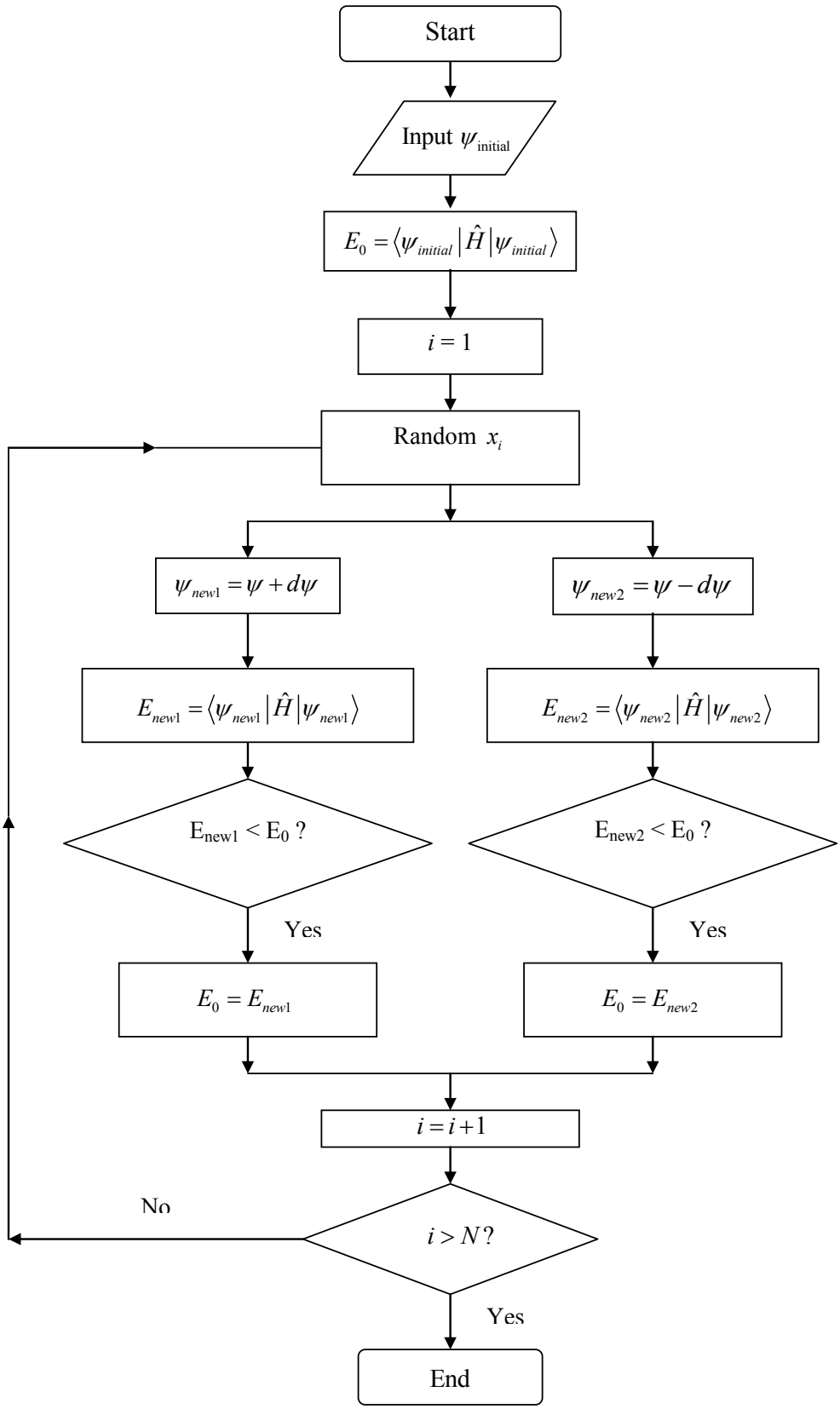


***Fig. 1*** Flow chart representing logic of this work.

*Table 1* Ground-state energies from VMC calculation compared with the ones obtained from Hill Determinant method.

| Parameters in case | $E_0$ from VMC | $E_0$ from Hill Det. | % difference |
|---|---|---|---|
| $\lambda = 1.0,\ k = 5.0$ | -3.38041 | -3.41014 | 0.87 |
| $\lambda = 1.0,\ k = 7.0$ | -8.67204 | -8.67111 | 0.01 |
| $\lambda = 1.0,\ k = 10.0$ | -20.63748 | -20.63358 | 0.02 |
| $\lambda = 6.0,\ k = 40.0$ | -57.98453 | -57.87859 | 0.18 |
| $\lambda = 0.5,\ k = 5.0$ | -9.37836 | -9.44698 | 0.73 |
| $\lambda = 1.5,\ k = 15.0$ | -32.10278 | -32.12731 | 0.08 |
| $\lambda = 5.0,\ k = 30.0$ | -37.34071 | -37.42980 | 0.24 |
| $\lambda = 10.0,\ k = 50.0$ | -52.70857 | -52.71005 | 0.003 |
| $\lambda = 15.0,\ k = 100.0$ | -152.83048 | -152.67831 | 0.10 |
| $\lambda = 25.0,\ k = 15.0$ | -208.17907 | -207.84995 | 0.16 |

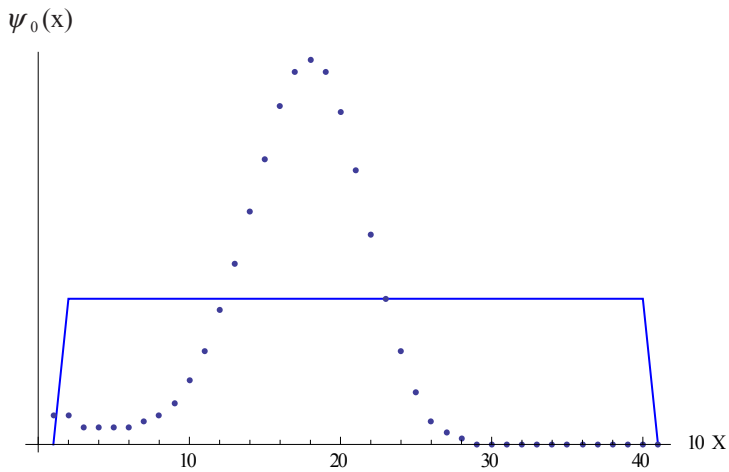


*Fig. 2* **Line** : Initial wave function via VMC in half domain (arbitrary units).
**Dot** : Final wave function calculated via VMC in half domain (arbitrary units).

*Ground-state wave functions*

After extended to full domain and rescaled, the wave functions are obtained as follows:

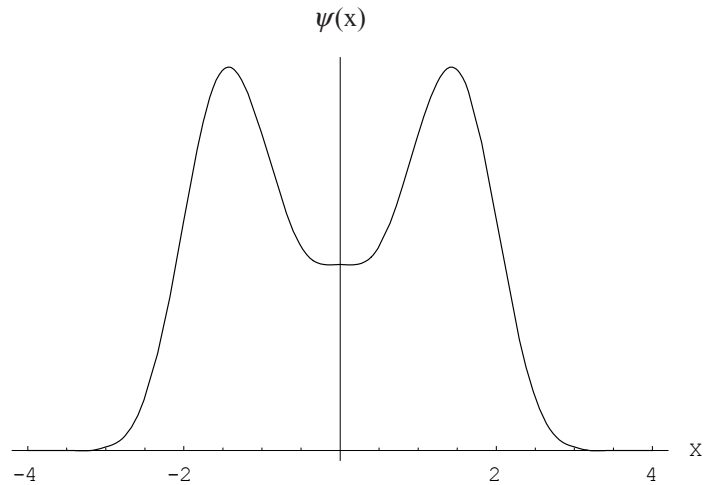


*Fig. 3* Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 1.0$, $k = 5.0$

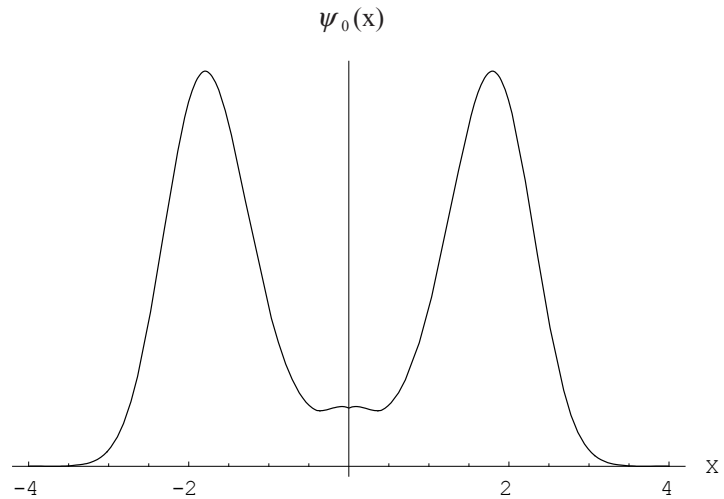


*Fig. 4* Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 1.0$, $k = 7.0$

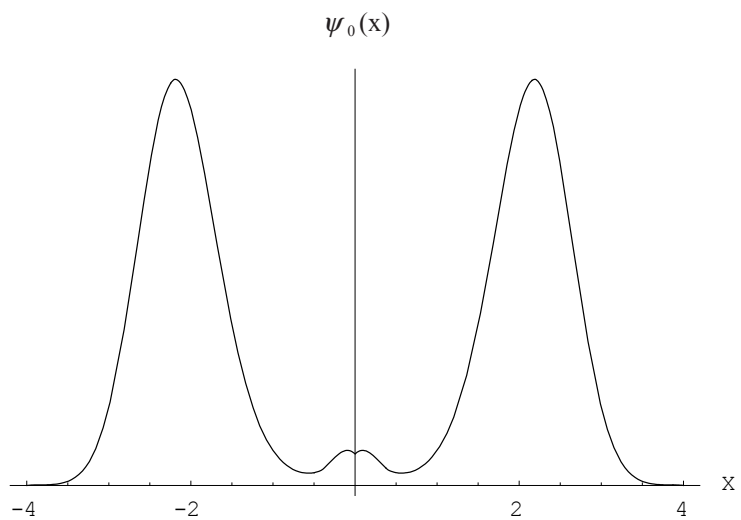


*Fig. 5* Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 1.0$, $k = 10.0$

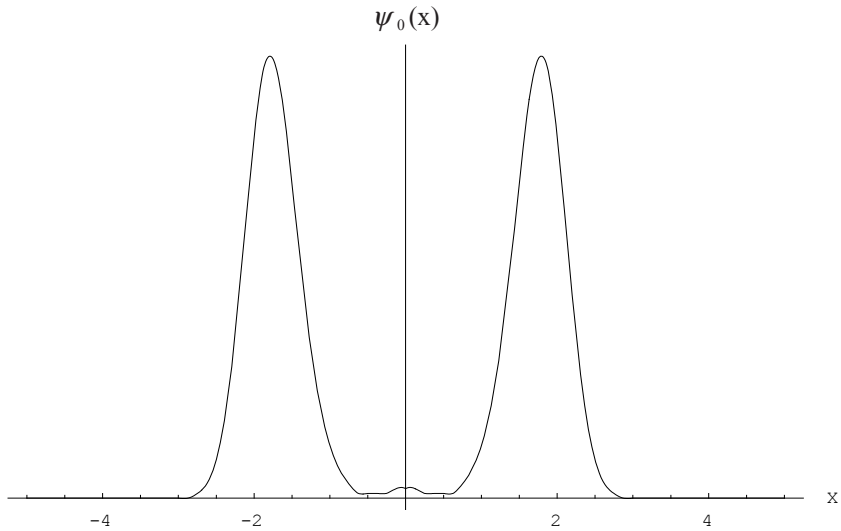


***Fig. 6*** Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 6.0$, $k = 40.0$

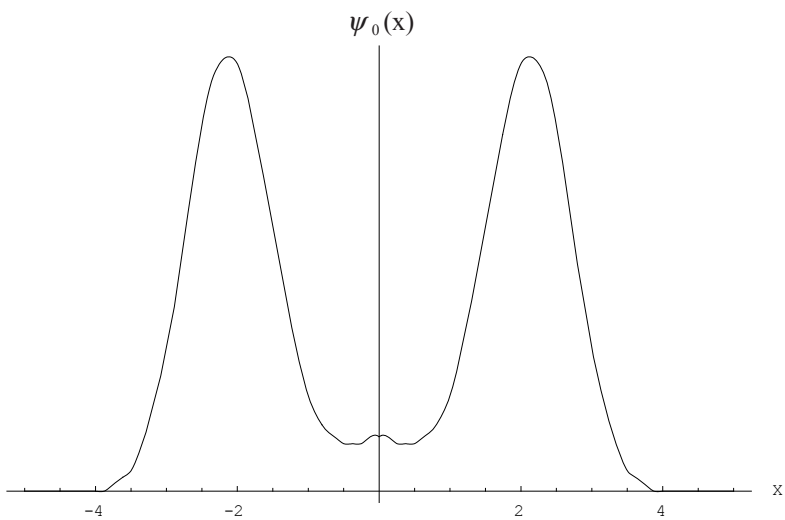


***Fig. 7*** Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 0.5$, $k = 5.0$

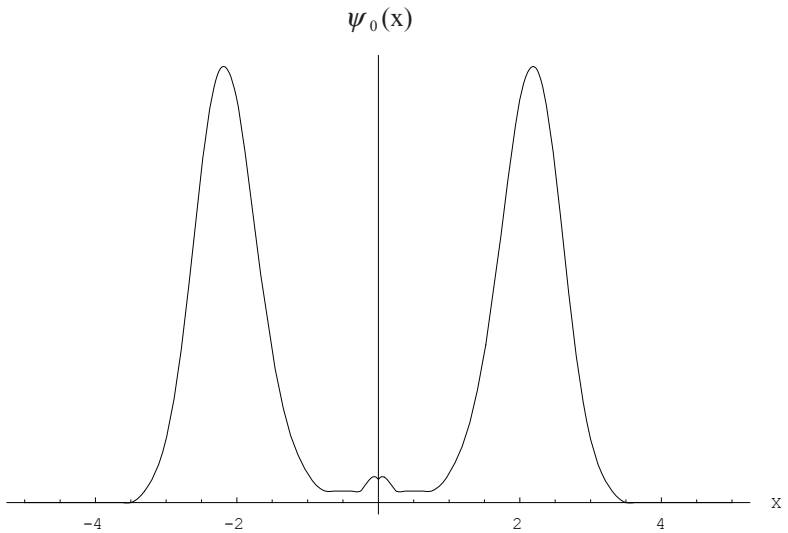


***Fig. 8*** Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 1.5$, $k = 15.0$

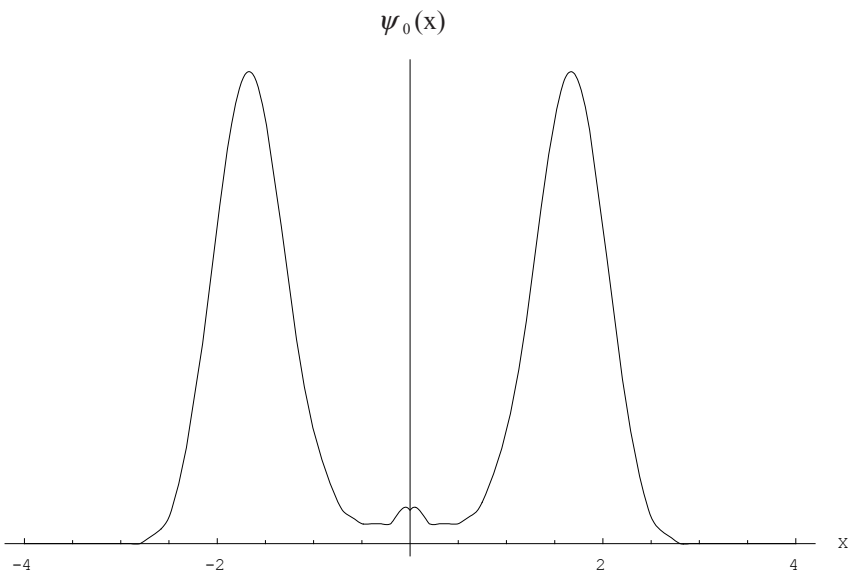


***Fig. 9*** Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 5.0$, $k = 30.0$

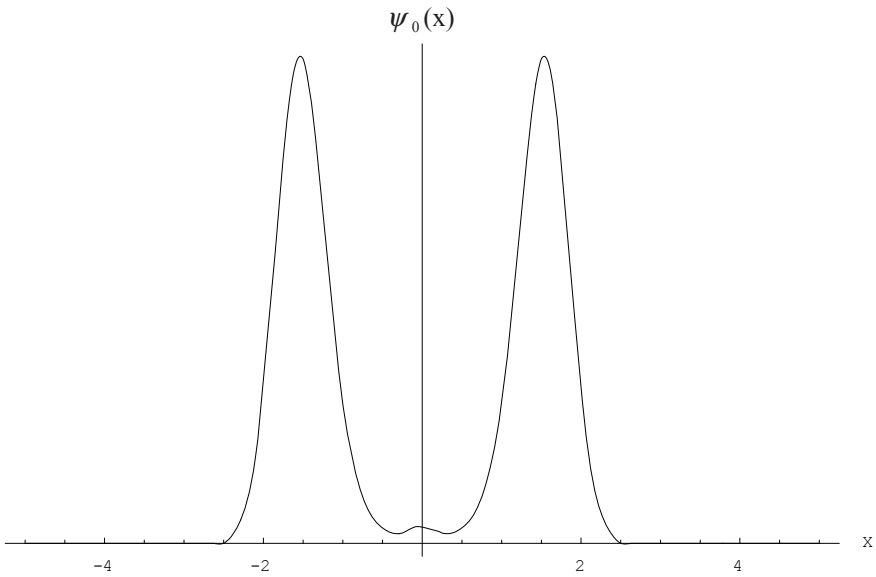


***Fig. 10*** Ground-state wave function via VMC, in arbitrary units, in case $\lambda = 10.0, k = 50.0$

## Conclusion

From the Monte Carlo principle, we have successfully adjusted the ground-state wave functions within the half domain by minimizing the energy eigenvalues. Due to the fact that the potential is an even function, then the wave functions are symmetric or antisymmetric. In other words, the ground-state wave functions of this problem must be even functions. Hence, using the half-domain technique reduces the computing time by about one half. We obtain numerical results of the energy eigenvalues in good agreement with those calculated via Hill-determinant method. This confirms the validity and correctness of random process.

By viewing the double well as a single well plus a central barrier, we know from elementary Calculus that the barrier width and height are $\sqrt{2k/\lambda}$ and $k^2$ / $(4\lambda)$ respectively. Therefore, the combination of $k$ and $\lambda$ determines the shape of double well. For example, for ground state in case of $k$ = 5.0, $\lambda$ = 1.0, the wave function decays noticeably as $x \to 0$ since the barrier in this case is pretty thin. The decay is, however, more obvious in case of $k$ = 30.0, $\lambda$ = 5.0 since the barrier gets thicker and the well gets deeper (the barrier height is higher). These results show that the graphs of wave function suit theoretical prediction indeed. Under this circumstance, we get closer level between $E_0$ and $E_1$ which, even though cannot be seen by this method (since this one normally deals with ground states), can somehow be observed from other means.

## Acknowledgements

I would like to thank the science faculty, Naresuan university for their financial support. Special thanks go to the Nicholas Giordano for his inspiring book computational physics that leads me to learn this technique.

## References

Arias de Saavedra, F. & Buenda, E. (1990). Perturbative-variational calculations in two-well anharmonic oscillators. *Physical Review A, 42*, 5073.

Balsa, R., Plo, M., Esteve, J.G. & Pacheco, A.F. (1983). Simple procedure to compute accurate energy levels of a double-well anharmonic oscillator. *Physical Review D, 28*, 1945.

Banerjee, K. (1978). General Anharmonic Oscillators. *Proceedings of the Royal Society A, 364*, 265.

Banerjee, K. & Bhatnagar, S.P. (1978). *Physical Review D, 18*, 4767.

Bansal, M., Srivastava, S. & Vishwamittar (1991). Energy eigenvalues of double-well oscillator with mixed quartic and sextic anharmonicities. *Physical Review A, 44*, 8012.

Bishop, R. F.& Flynn, M. F. (1988). Variational and coupled-cluster calculations of the spectra of anharmonic oscillators. *Physical Review A, 38*, 2211.

Biswas, S.N., Datta, K., Saxena, R.P., Srivastava, P.K. & Varma V.S. (1973). Eigenvalues of $kx^{2m}$ anharmonic oscillators. *Journal of Mathematical Physics, 14*, 1190.

Brickmann, J. & Zimmermann, H. (1969) Lingering time of the proton in the wells of doubleminimum potential of hydrogen bonds. *Journal of Chemical Physics, 50*, 1608.

Chaudhuri, R. N. (1985). Comment on the anharmonic oscillator and the analytic theory of continued fractions. *Physical Review D, 31*, 2687.

Drozdov, A.N. (1995). On the improvement of convergence of Hill determinants. *Journal of Physics A., 28*, 445.

Fernandez, F.M., Meson, A.M. & Castro, E.A. (1985). A simple iterative solution of the Schroedinger equation in matrix representation form. *Journal of Physics A:* Math. Gen., *18*, 1389.

Flessas, G.P. (1979). On the eigenvalues of the rotating harmonic oscillator. *Physics Letters A, 71*, 315.

Flessas, G.P. & Anagnostatos, G.S. (1982). On the applicability of the Hill determinant and the analytic continued fraction method to anharmonic oscillators. *Journal of Physics A, 15*, L537.

Friedburg, R., Lee, T.D., Zhao, W.Q.& Cimenser, A. (2001). A convergent iterative solution of the quantum double-well potential. *Annals of Physics, 294*, ISSUE1.

Fröman N., Fröman, P.O. & Karlsson, F. (1980). Comments on a paper concerning the eigenvalues of the rotating harmonic oscillator. *Physics Letters A, 77*, 397.

Gerald, C.F. & Wheatley, P.O. (2004). *Applied Numerical Analysis* (7E), Boston:Pearson-Addison.

Handy, C. R. (1992). Application of the eigenvalue moment method to the quartic anharmonic double-well oscillator. *Physical Review A, 46*, 1663.

Hautot, A. (1981). Interaction $kx^2 / (1 + gx^2)$ revisited. *Journal of Computational Physics, 39*, 72.

Hautot, A. (1986). On the Hill-determinant method. *Physical Review D, 33*, 437.

Hautot, A. & Magnus, A. (1979). Calculation of the eigenvalues of Schroedinger equations by an extension of Hill's method. *Journal of Computational Applied Mathematics, 5*, 3.

Hautot, A. & Nicolas, M. (1983). On the applicability of the Hill-determinant method. *Journal of Physics A., 16*, 2953.

Hodgson, R.J.W. (1989). Splitting in a double minimum potential with almost twofold degenerate lower levels. *Journal of Physics A: Math.Gen., 22*, 61.

Killingbeck, J. (1986). Hill determinants and supersymmetry. *Physics Letters A, 115*, 253.

Ram-Mohan, L.R. (2002). *Finite Element and Boundary Element Applications in Quantum Mechanics*, Oxford:Oxford University Press.

Reddy, J.N. (1993). *Introduction to the Finite Element Method* (2E), New York:McGraw Hill.

Schiffrer, G. (1985). Improved calculations of anharmonic oscillators using the gradient method. *Nuovo Cimento B, 90*, 74.

Somorjai, R.L. & Hornig, D.F. (1962). Double-minimum potentials in hydrogen-bonded solids. *Journal of Chemical Physics, 36*, 1980.

Tater, M. & Turbiner, A.V. (1993). Failure of the Hill determinant method for the sextic anharmonic oscillator. *Journal of Physics A., 26*, 697.

Witwit, M.R.M. (1996). Energy levels for nonsymmetric double well potentials in several dimensions: Hill determinant approach. *Journal of Computational Physics, 123*, 369.

Witwit, M.R.M. & Killingbeck, J.P. (1993). Hypervirial perturbation calculations for doublewell potentials of perturbed oscillator type. *Canadian Journal of Physics, 71*, 475.

Zhou, F., Cao, Z. & Shen, Q. (2003). Energy splitting in symmetric double-well potentials. *Physical Review A, 67*, 062112.

Zienkiewicz, O.C. & Morgan, K. (1983). *Finite Elements and Approximation*, London:Wiley.

Znojil, M. (1982). Comment on the Green's function for the anharmonic oscillators. *Physical Review D, 26*, 3750.

Znojil, M. (1986). Polynomial potentials and a hidden symmetry of the Hill-determinant eigenvalue method. *Physics Letters A, 116*, 207.

Znojil, M. (1988). On the power series construction of bound states I. The energies as zeros of the infinite Hill determinants. *Journal of Mathematical Physics, 30*, 1433.

Chaiharn, J. (2008). *Finite Element Treatment of Quantum Mechanical Quartic Double-Well Potential Problem*, Master's Thesis, Graduate School, Naresuan University.

Wan-ek, A. (2008). *Application of Numerical Shooting Method to Quantum Mechanical Quartic Double-Well Potential Problem*, Master's Thesis, Graduate School, Naresuan University.