Theoretical and computational study of quantum Systems Optimization for Ground State Energies

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Abstract: In this article tried to study about the novel optimization method to calculate the Ground State Energies in spherical quantum centre. In this regard, various functions are considered for ground state and then ground state energies will be calculated. Finally, optimization method is used for energies optimization to achieve final result. Optimization method in this research has been used to provide ground state energy of a quantum system in spherical coordinates. Optimization method is based on applying evolutionary operators such as crossover, mutation and reproduction (copy) on primary population and used for quantum problems as well as for engineering issues. Both methods; parameter optimization and wave function are compared here for optimization problems to calculate eigenvalues of energy. The results of this method are in agreement with trial values. It must be noted that Matlab software has been applied for all physics and quantum computations. Therefore, the comparison between the results and exact values of theory in this method indicated that this method in comparison with other methods is significantly accurate.

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1. Introduction

Optimization is a new phase of intelligent optimization methods and is available to optimize different engineering issues and other sciences. Using optimization method based on evolutionary computation, solving problems are used in the nonlinear and multidimensional spaces with high speed and efficiency, especially in solving some problems in quantum physics. To date, the study of semiconductor nanostructures has been based on numerical and variable methods [1].

Recently, optimality method as a different optimization method is used for optimization issues of quantum systems significantly [5,18]. This method proposed by Holland [5] has been used for various fields included engineering, optimization problems, computing energy for atomic and molecular physics as well as the study of crystal growth in condensed matter. The method principles are similar to variational method. The differences between them are described as following:

1.use codes instead of parameters in a problem.
2 .start with each possible primary population.
3.no derivation or other auxiliary information used by this process.
4.use probabilistic rules, not determined.

The general procedure of optimality is to produce next population among primary population of possible solutions based on a series of predetermined selection rules. Individuals' fitness is a main criterion for next phase. So, lower fitness led to remove individuals. Fitness, in second phase, is higher for selective population. Crossover and mutation are done based on predetermined probability from selection phase. The work mentioned steps are repeated sequentially led to produce population with higher fitness. This work will be continued to predetermined convergence or limit.

For each quantum system, optimality method is used first through trial selection of ground state wave function and after computing their energy, fitness will be considered for each of them (fitness is computed based on minimizing the energy). Crossover and mutation will be repeated to achieve acceptable result during selection phase

The purpose of this article is to obtain ground state energy of a quantum system and in this regard, different methods included optimization method based on parameters optimization and based on wave function optimization will be used. The results indicated that optimization based on wave function to present physics results is more accurate than other methods. Optimization method in this research is used for optimality for impurity problem in center of spherical quantum dot with infinite

limited potential. There are two different processes to apply optimality method in this problem. Finally, the results are compared with the results of the proposed method.

2. Study of common optimization methods

Optimization of variational method:

In a system, eigenvalue of energy is very low for ground state,

$H|0\rangle = E_0|0\rangle$

but, energy is high for other states,

$H|n\rangle = E_n|0\rangle, \qquad E_n > E_0$

It is not possible to solve eigenstates and eigenvalues significantly by a Hamiltonian. Ground state seems is similar to |˜0i. Two words "ansatz" or "trial" wave function is used instead of "guess" among many scientists. A guess is a guess. The ansatz is a linear combination of different Hamiltonian eigenstates, if it is incorrect.

$$|\tilde{0}\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\tilde{0}\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$$

If c_0=1 and c_n=0 for all n≠ 0, ansatz is right. Normalization needs

$|c_0|^2 + \sum_{n\neq 0} |c_n|^2 = 1$

The energy value expected for ansatz is as following:

$$\langle\tilde{0}|H|\tilde{0}\rangle = |c_0|^2 E_0 + \sum_{n\neq 0} |c_n|^2 E_n \geq |c_0|^2 E_0 + \sum_{n\neq 0} |c_n|^2 E_0 = E_0$$

In this regard, the ground state energy always needs to greater or equal energy value. Using arbitrary trial ket, upper limit on the ground state energy eigenvalue will be achieved. It is obvious that higher trial ket can lead to higher upper limit and higher overlap with the real ground state will occur. In other word, lower Hamiltonian value of state can also lead to true ground state with higher overlap. In this regard, energy value of trial ket is computed by parameters to the $|\tilde{0}(\lambda_1, \lambda_2, \cdots)\rangle$ for ground state wave function.

$$\bar{E}(\lambda_1, \lambda_2, \cdots) = \langle\tilde{0}(\lambda_1, \lambda_2, \cdots)|H|\tilde{0}(\lambda_1, \lambda_2, \cdots)\rangle$$

Low value expected needs to minimize as following:

$$\frac{\partial \bar{E}}{\partial \lambda_1} = \frac{\partial \bar{E}}{\partial \lambda_2} = \cdots = 0$$

There is a relationship between better parameters and better trial ket can lead to the method success. It is known as variational method. In this way, the differences will find in parameters within ansatz and lower energy value will occur. Lower energy value depends on the more close relationship between the ansatz and true ground state. In other word, true ground state occurs by true functional form of ansatz.

Hamiltonian for a quantum system in ground state is as following:

$$H = \frac{-\hbar^2}{8\pi^2 m}\nabla_r^2 - \frac{e^2}{r} + V(r)$$

where ∇^2 is Laplacian in Spherical coordinates.

$$\nabla_r^2 = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}$$

According to that, V(r) is potential, e is electron charge and m is electron mass and all values are considered in selective units [16]. The ground state energy of system will be obtained through solving equation.

$$(H - E_n)\ \psi_n = 0$$

There are different methods for solving this equation included perturbative method [4], variational method [2 &3] and/or numerical solution [17].

According to this article, wave function that describes the system is defined as a 3-dimensional sphere of radius R as following:

$$\psi_r = \begin{cases} A\dfrac{\sin(kr)}{r}\exp(-\lambda r) & r < R \\ 0 & r > R \end{cases}$$

where $k = \frac{\pi}{R}$ *and* λ *are true parameters. Coefficient A is obtained from normalization process.*

$$V(r) = \begin{cases} 0 & r < R \\ \infty & r > R \end{cases}$$

Parameter optimization:

The parameter optimization is a general method [6&7] that inspired by the evolutionary process in nature. This method is through primary population of individuals presented as chromosome. During this method, individuals are changed and each phase is contained optimization information of previous phase. But, objective new phase involves significant values of the objective function rather than previous phase. When the value of objective function was computed for each of the population individuals, 3 main operators in this method are usable for population, they are respectively as following:

1.Reproduction (copy)
2.Crossover
3. Mutation

In reproduction process, there are different selection methods such as revolving wheel [8], ranking and … and individuals are selected through

the optimal value of the objective function and reproduced to next phase .

In crossover, two individuals are selected randomly from current population and they replaced their components together by cutting out of random point. Sometimes, the process of searching occurs in local optimum and leads to mutation process in order to get out of local optimum. However, crossover operator with lower percentage in comparison to mutation process is used in mechanism of the method. And mutation can lead to random change for optimization of the problem information. Reproduction, crossword and mutation are done for each phase of optimization process on individuals and all phases will be repeated for several times for optimal result.

In order to apply the optimality, it is required to know which parameter should optimize for each physics problem. Primary value of energy is calculated by following equation.

$$E = \min_{\lambda} \frac{\langle \psi^*(\lambda, r) | H | \psi(\lambda, r) \rangle}{\langle \psi^*(\lambda, r) | \psi(\lambda, r) \rangle}$$

Now, the value of competency for each of primary population is shown by following equation.

$$\text{Fitness}[\psi_i] = \exp[-\beta(E_i - |E_{av}|)]$$

According to that, β is constant number. Selection phase is done through computing the fitness and higher fitness will be produced for next phase [9]. In crossover, primary population ofλ should be changed into binary codes and two of them (parents) with predetermined probability which randomly selected from a point, both halved and their second half will be replaced together in order to produce a new element (child). In next phase (mutation), A binary string of predetermined probability (and much less likely to crossover) is selected and one of their information will be changed randomly. Above phases will be repeated to achieve perfect result.

Optimization of the wave function:

Wave functions in this method are selected as optimality codes and optimality operations directly will be done on them. Hence, primary population will be produced and as previous method, next population will be selected through computing the individuals' fitness. Two wave functions are selected for crossover of wave function (parents) and new wave functions will be produced as following:

$$\psi_1'(r) = \psi_1(r)S(r) + \psi_2(r)[1 - S(r)]$$

$$\psi_2'(r) = \psi_2(r)S(r) + \psi_1(r)[1 - S(r)]$$

Here, S(r) can be used as following:

$$S(r) = \frac{1}{2}\left[1 + \tanh\left((r - r_0)/w^2\right)\right]$$

Where r0 is each random number between the interval (0,R). W is a determiner parameter of crossover intensity [7]. The probability of crossover was equal to 95% for each optimality phase. Two number of wave function are selected randomly from produced population in crossover and new member will be produced by them:

$$\psi'(r) = \psi(r) + \psi_M(r)$$

Lower probability of mutation should be selected, means 0.05%.

In this method, the number of primary population is constant to reach the results of above phases. In this regard, wave function is considered as optimization code instead of variational parameter. First, a primary population is produced based on random values of contained N of wave function. This population will be normalized. So, first phase is a normalized population of wave function. The obtained result of objective function value caused to produce a new population based on optimization operators and selection process is done by revolving wheel method. Then, reproduction operator is done for population in order to copy some individuals with higher objective function value to next phase and remove individuals with non-appropriate objective function. Hence, uncertain crossover which wave functions have been selected randomly and new wave functions will be used. The main purpose to use of uncertain crossover is to prevent large differences between the wave functions of different phases. Small variational values for a function can raise the possibility of discontinuity, so accuracy is very important issue for mutation operation. It is unacceptable by physics. Therefore, an arbitrary Gaussian distribution can use as mutation function to prevent discontinuity. Then, mutation operator will be applied. This process will be repeated until the results of system ground state wave function to be achieved.

3. Proposed method

Trial wave function ϕ(λ1, λ2, . . . , λn) leads to mean energy of quantum state as following:

$$\bar{E}(\lambda_1, \lambda_2, \ldots, \lambda_n) = \frac{\int \Phi^* \hat{H} \Phi \, d\tau}{\int \Phi^* \Phi \, d\tau} \geq E_0 ,$$

According to that, variational parameters are λi, (i = 1, . . . , n) and ground state energy of the quantum state is E_0. $\bar{E}$ ($\lambda_1, \lambda_2, \ldots, \lambda_n$) is as lower mean energy of some variational parameters for ground state energy. There is a relationship between multidimensional unconstrained optimization problems and ground state energy. In optimization

problems, cost function is mean energy $\bar{E}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and optimal design parameters is variational parameters $\lambda_1, \lambda_2, \ldots, \lambda_n$. Vector $S = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ is shown. Thus, lowering the mean energy E(S) is a main purpose that can be done by setting S.

Representation of Chromosomes: in the mean energy E, all the variational parameters λ1, λ2, . . . ,λn are chromosome's components.

Fitness: in order to minimize $\bar{E}$, it requires to find parameter set $S = (\lambda_1, \lambda_2, \ldots, \lambda_n)$. F is introduced as fitness function by following equation:

$$F(\lambda) = C - \bar{E}(\lambda),$$

That, C is equal to 10000 and is as a larger positive number. Also, F(λ) → maximum as $\bar{E}(\lambda)$ → E0.

Selection: in this method, the purpose is to produce "child" chromosomes by "parent" individuals. First, computing the objective function value is essential for each individual. The size of population has impact on the method repetition.

Crossover: in this method, each child produces by combination of two parents' genes. Assume that two vectors; $A = (A_1, A_2, \ldots, A_n)$ and $B = (B_1, B_2, \ldots, B_n)$ show the region of variational parameters; $Ai \leq Si \leq Bi$ (i = 1, 2, . . . , n) and two chromosomes; So1i and S_{o2i},are selected for crossover application. So, So1i ≤ So2i. According to following, a child S_{ni} will be produced:

If (θ % 3) = 0 then $S_{ni} = {}_{\alpha}A_i + (1-\alpha)S_{o1i}$
If (θ % 3) = 1 then $S_{ni} = {}_{\alpha}S_{o1i} + (1-\alpha)S_{o2i}$
If (θ % 3) = 2 then $S_{ni} = {}_{\alpha}S_{o2i} + (1-\alpha)B_i$

That, random number is α ε [0, 1] and random integer is θ 0. When parents are located contrary to the hill, some searches will be done for hill climbing with high convergence speed to determine a genetic algorithm.

Mutation: assume that we have a chromosome is called S = (λ1, λ2, . . . ,λn) and a mutant gene is called Si 2 [ai, bi]. Following equation is related to apply various mutation operators (here, mutation operator is Improved Gaussian), i.e, the gene S0 i.

$$S_i' = S_i + \sigma\left(\sum_{j=1}^{12} r_j - 6\right),$$

that, random number is (0,1) and σ = 1/6. Local area surrounding the primary individual has been determined by mutation operator.

Stopping Criteria of the Algorithm: the higher value of individual's fitness and production all generations can lead to stop algorithm.

4. Results and discussion

The results are shown in figure 1 to compare with exact values and the results of variational method [3, 14]. Atomic units used for all computations. Optimality efficiency is determined based on figure 1. The results of wave function optimization are more exact than the results of variational method. The variational parameters values of λ are computed based on variational and optimization methods by optimality are shown in figure 2. For many years, variational method is used for practical problems. So, applying the variational method is more difficult, if the number of variational parameters become more than one. Additionally, variational method is more sensitive than selecting primary functions and parameters. But, optimality method is less sensitive than starting point and complexity of the problem.

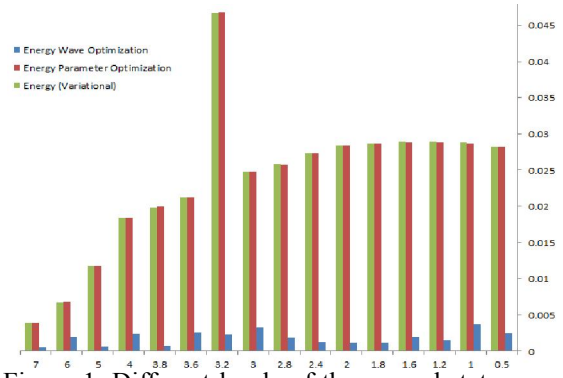

Figure 1. Different levels of the ground state energy as a function of the radius of the quantum dot like three previous methods hill climbing with high convergence speed to determine a genetic algorithm.

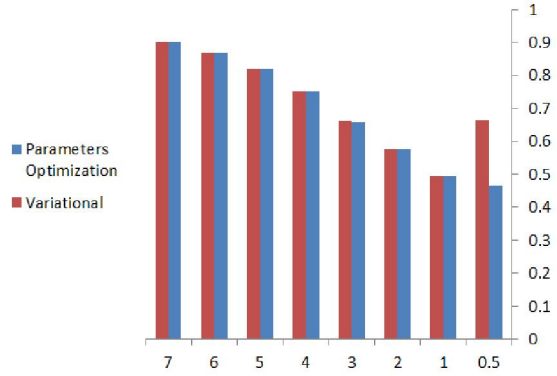

Figure 2. the values of variational parameters of λ based on variational and parameter optimization methods for optimality

The results of optimality method is shown in figure 3 based on wave optimization and exact values of energy and proposed method by Rydberg calculations. The energy values are extracted exactly by reference and all energy values are provided based on Matlab programming. Here, selective units [1] are used and also $h=m_e=e=1$. As shown in figure, the

results of proposed optimization method are closer to exact values than wave optimization.

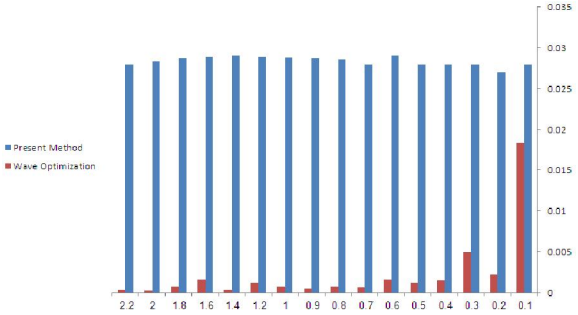

Figure 3. Different levels of the ground state energy in comparison of proposed method with wave function as a better method

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