

Review

A new approach based on genetic algorithm in Schrödinger equation solution for nanostructure applications, the effect of some genetic and Monte Carlo operators

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In this work, we have developed our previous work which combines the genetic algorithm, Monte Carlo and variational methods (GMV). Some new facts about the application of the method are revealed. In order to illustrate the Fmethod, the diamagnetic shift and the effect of the barrier thickness on the exciton binding energy of the GaAs_{0.7}Sb_{0.3}/GaAs single quantum well (GW) are described.

Key words: Monte Carlo integration scheme, genetic algorithm, variational method, hybrid method, quantum well, diamagnetic shift.

INTRODUCTION

During the last decades, different computational methods have been devised to solve the single and many particle Schrödinger equations. Among these vast number of computational methods finite-difference time-domain (Boykin et al., 2002), random walk (Crow et al., 1999), genetic algorithm (Solaimani et al., 2010), density matrix renormalization group (Duque et al., 2008), variational method (Escorcia et al., 2004), perturbation approach (Fu et al., 2006), Monte Carlo method (Arabshahi, 2011), power series expansion (Juri and Tamborena, 2005) and the exact solution (Lin, 1989), 1/N expansion methods (Golafroz and Arabshahi, 2010), asymptotic iteration method (Zhu and Huang, 1987) and finite element method (Wei, 1989) are among the methods which are used in the literatures to investigate the nanostructures.

Among these different methods, matching methods are not well suited to satisfy boundary conditions at more than one point and, therefore, cannot easily be used in two or three dimensions. A general method for dealing with these cases is to write the Schrödinger equation in the form of a matrix eigenvalue problem. Such

approaches are computationally very difficult to carry through, and in application to higher degrees of freedom, the computational cost will also grow exponentially.

Application of the genetic algorithm to find best variational parameters is done several times till now (Soylu and Boztosun, 2008), but a study of the components of the genetic algorithm on a physical quantity is not done. As we have shown in our previous works (Oettinger et al., 1995) using a wrong procedure in the application of the genetic algorithm may lead to an un-meaningful physical result. Our other aim was to present a powerful method to solve many particles Schrodinger equation faster than the usual method, but at first we started with a two particle problem (an excitonic model) and tested its different part in a physical quantity like diamagnetic shift (e.g. mutation probability) to be able to open a new way.

The effect of the confinement on impurity and exciton have been studied vastly during the past years (Mann et al., 1984) and thus, much experimental and theoretical works have been devoted to the quantitative understanding of the physical properties of shallow impurities and excitons in single QW's specially in GaAs based ones. GaAs has special properties which enable it to be used in technology of infrared photodetectors,

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diodes, quantum well lasers, transistor, quantum well waveguides, etc. Exciton binding energy of this material in the form of a quantum structure like quantum wells is also having attracted great interest, thus we have selected a different doping GaAs_{0.7}Sb_{0.3}/GaAs as our target quantum well structures.

Here, we have introduced some other aspects of our recently introduced GMV method which we have demonstrated its validity in our previous works. Two of its advantages are that the computational cost management and the boundary condition implementation in more degrees of freedom are not so complicated. In application to a single quantum well GaAs_{0.7}Sb_{0.3}/GaAs we have extracted the diamagnetic shift as a function of magnetic field. Some components of the Genetic algorithm like mutation probability, population number, number of Genetic iteration, number of mesh points in Monte Carlo integration and also the effect of the barrier thickness on the exciton binding energy is investigated in order to find the right method in applying the genetic algorithm which is the main goal of this work.

THEORY

The main steps in this work are the same with our previous papers (Makino et al., 2006) which uses the simple variational scheme that exploits the ground states energy and eigenfunction of an arbitrary quantum system:

$$E_0 = \min \int \psi^* H \psi dr \quad (1)$$

where ψ is a trial normalized wave-function. In order to describe the method, we have applied it to a symmetric single quantum well to investigate the diamagnetic shift and exciton binding energy. For this purpose, and for simplicity of comparing our results, we have used again the Hamiltonian of the Senger (Hilton et al., 1992),

$$H = \sum_{i=e,h} \left(-\frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial z_i^2} + V_i^{conf}(z_i) \right) - \frac{\hbar^2}{2\mu} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{e^2}{\epsilon_0 \sqrt{\rho^2 + (z_e - z_h)^2}} + \frac{1}{8} \mu \alpha^2 \rho^2 \quad (2)$$

with the trial wave function,

$$\psi(\vec{r}_e, \vec{r}_h) = f_e(z_e) f_h(z_h) \exp(-\lambda \sqrt{\rho^2 + a^2(z_e - z_h)^2}) \times \exp(-b^2 \rho^2) \quad (3)$$

where $f_i(z_{i=e,h})$ are the envelop functions, of which e and h indicate the electron and hole. The frequency is

$\omega = \frac{eB}{\mu c}$, where e is the free electron electrical charge, B is the magnetic field, c is the speed of light in vacuum, and the reduced mass is $\mu = (1/m_e + (\gamma_1 + \gamma_2)/m_0)^{-1}$, where γ_1 and γ_2 are the Kohn-Luttinger band parameters which is the same as that used in Senger. λ , a and b are the free parameters of this trial Wave function that can be found by the minimization of

$E_0(B) = \min_{a,b,\lambda} \langle \psi | H | \psi \rangle$. Now the diamagnetic shift is simply defined as $\delta = E_0(B) - E_0(B=0)$. The exciton binding energy is also defined as $E_b = E_g + E_e + E_h - E_{ex}$, where E_g is the energy gap, E_e and E_h are computed by using,

$$\left[\frac{E_e}{V_e} \right]^{1/2} = \cos \left[\left[\frac{m_e E_e}{2\hbar^2} \right]^{1/2} L \right] \left[\frac{E_h}{V_h} \right]^{1/2} = \cos \left[\left[\frac{m_h E_h}{2\hbar^2} \right]^{1/2} L \right] \quad (4)$$

which we have solved by using Bisection method. E_{ex} is defined as it is presented in Equation 1. We have used the Ben-Daniel-Duke boundary condition in order to include the effect of the effective mass mismatch in the well and barrier. We have also used the Vigar law to find the effective mass of the electron and hole in the well.

RESULTS AND DISCUSSION

We have investigated some components of a previously introduced method which was a combination of the genetic algorithm, variational method and Monte Carlo integration scheme (GMV method) like mutation probability, population number, number of genetic iteration, number of mesh points in Monte Carlo integration and exciton binding energy, when we applied it to a single quantum well GaAs_{0.7}Sb_{0.3}/GaAs.

We have obtained Figure 1 which shows the variation of the diamagnetic shift as a function of the mutation probability and the applied magnetic field in a 3D plot. As the Figure 1 shows, there is an oscillatory aspect in terms of the mutation probability thus, it is not reasonable to use an arbitrary mutation probability to find the diamagnetic shift. Note that in our application the mutation probability is used by turning small values of a member of population to large ones and vice versa. However, we have used a criterion to find the best mutation probability. The best mutation probability is one which leads to the smallest value for the ground state energy.

Variation of the diamagnetic shift as a function of the number of genetic iterations in Figure 2 shows an oscillatory behavior. This means that, small numbers of iterations are needed to find a good approximation for the free parameters in our variation scheme and also, this means that the typical type of the selected trial wave function is similar to the original wave function of the problem. This wave function was previously selected with some physical intuitions, but now we proved it by our GMV implementation. Now, the oscillatory behavior with respect to the number of genetic iterations is due to the stochastic nature of the GA method, and now the problem is to find some techniques to reduce the amount of oscillation around the real value. Another result which is not so strange is that an increase in the number of population numbers in a fixed higher number of genetic iterations always does not lead to a accuracy, but it only oscillates around the real value which is presented in the

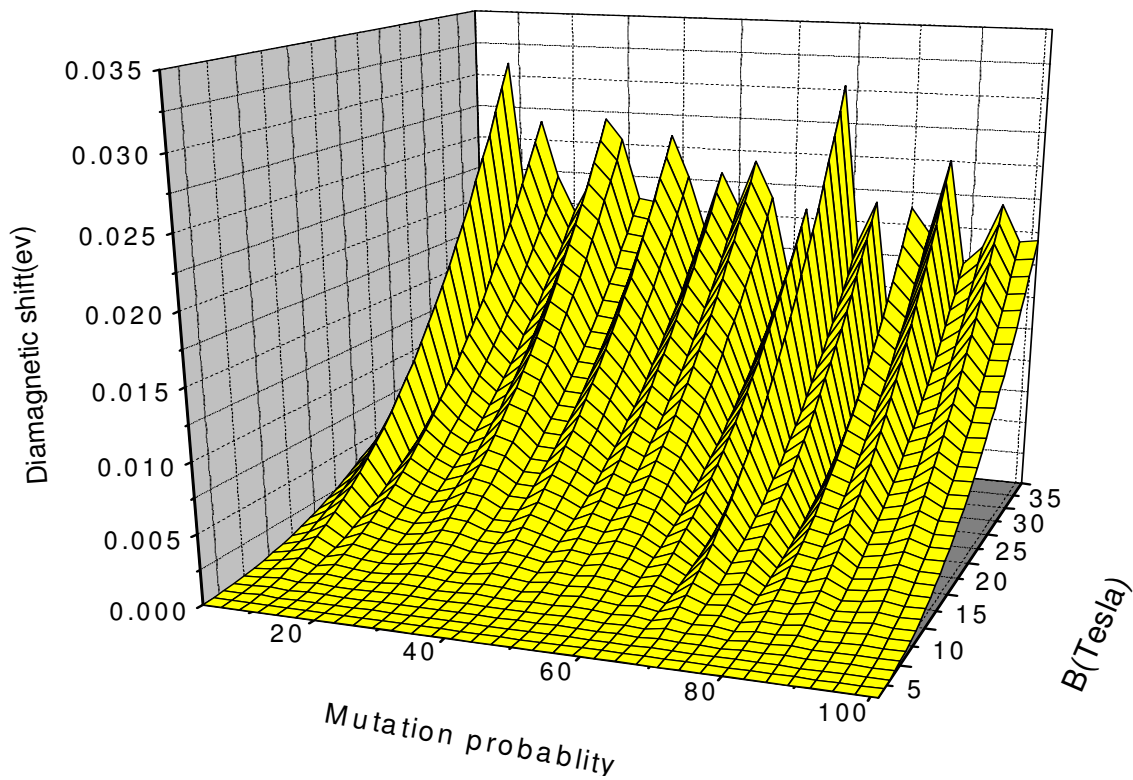


Figure 1. Diamagnetic shift as a function of mutation probability and the applied magnetic field B (in Tesla).

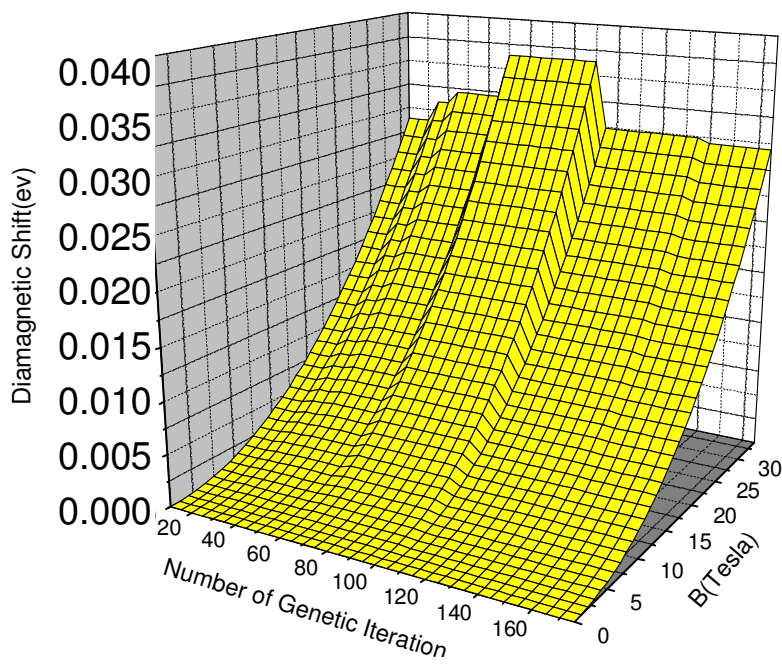


Figure 2. Diamagnetic shift as a function of magnetic field and number of genetic iteration.

Figure 3. This figure shows the 3D plot of variation of the diamagnetic shift as a function of the population number

and magnetic field B which has an oscillatory behavior. This is a useful finding, because now we use smaller

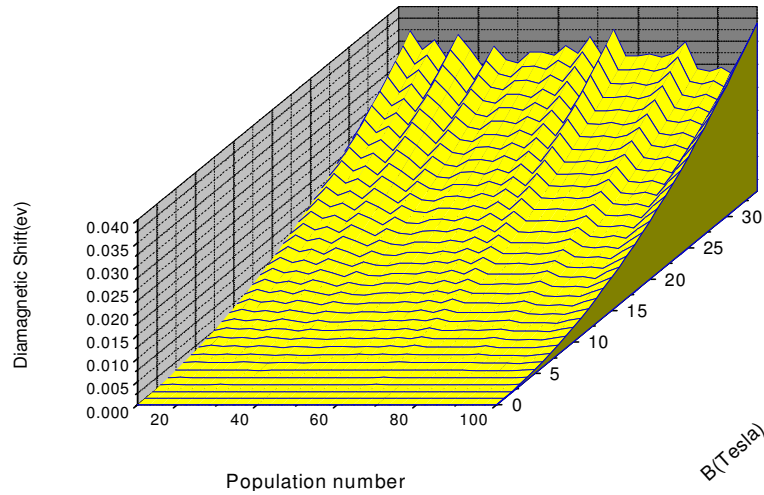


Figure 3. Diamagnetic shift as a function of population number and magnetic field B at maximum genetic iteration 100.

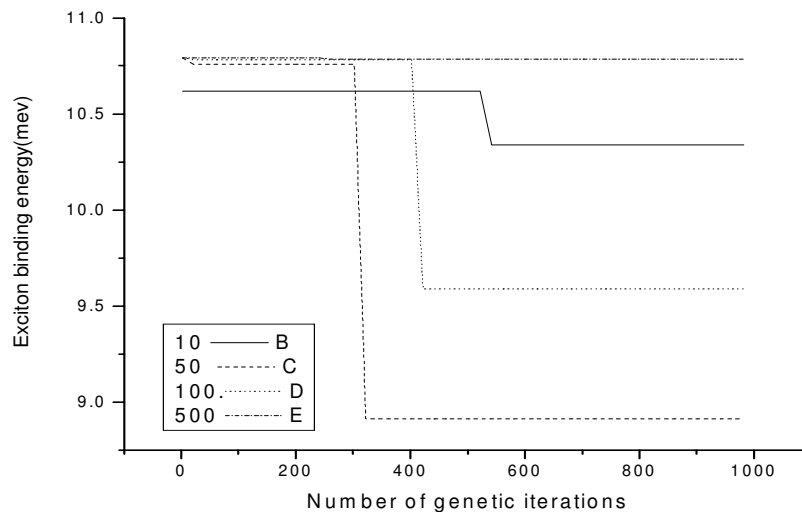


Figure 4. Ground state expectation value of the Hamiltonian 1 for different values of the Monte Carlo integration mesh points.

number of population number and try to find some schemes which reduce the amount of oscillation around the exact value of the typical physical quantity, and if we could not find such a scheme we can use the averaging procedure. This works are among the future works we want to do. The effect of one of the genetic algorithm components, that is, population number and mutation probability is small at low magnetic field, but by an increase in it, these effects are more visible (amount of oscillation). Figure 4 shows the effect of the number of mesh points in the Monte Carlo integration.

As it shows, by increasing this number the ground state energy saturates in different levels. This investigation is required to find the smallest value which leads to the correct ground state energy and do not waste too much

time to find other physical quantities which we want to calculate. To find this diagram we have assumed that the electron and hole can infinitely tunnel in the barrier region in order to investigate the effect of the barrier length. Another fact is that with an increase in the number of mesh points in the Monte Carlo integration, the diagram has reached to the minimum energy that does not saturate in a smaller energy. This is because with much number of Monte Carlo mesh points, the statistical average is closer to the real value of the integral and this is a statistical behavior. In Figure 5, variation of the exciton binding energy as a function of the well width for different barrier thickness, 30, 5000, 1000, 2000 and infinity is presented. For compression purposes we have plotted the exciton binding energy (Greene et al., 1985). The most

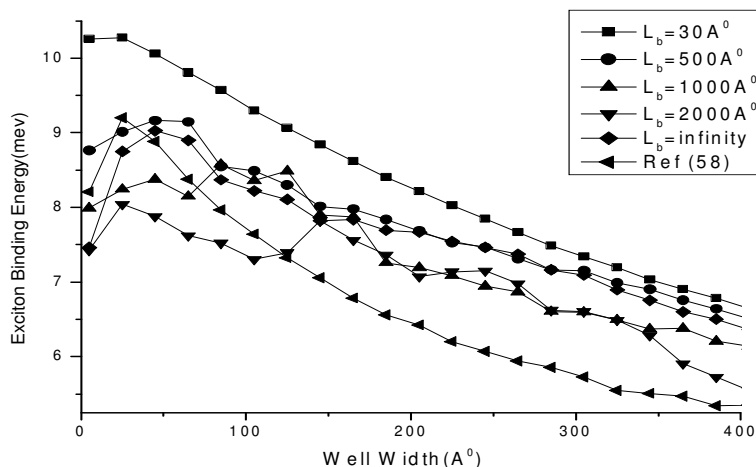


Figure 5. Variation of the exciton binding energy as a function of the barrier thickness for different well width.

agreement is achieved with the previous work when we used the infinity as the barrier thickness.

In summary, we have investigated some components of a hybrid method based on genetic algorithm which uses variational and Monte Carlo schemes (GMV method). For illustration purposes, we have applied the method to a GaAs_{0.7}Sb_{0.3}/GaAs single quantum well and extracted the diamagnetic shift as a function of magnetic field, exciton binding energy as a function of the barrier thickness for different well width, mutation probability, population number, number of genetic iteration and number of mesh points in Monte Carlo integration. It is proved that when one uses genetic algorithm to investigate some problem, investigating the genetic algorithm and Monte Carlo components like mutation probability, population number and number of mesh points in Monte Carlo integration may help to find the results more quickly.

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