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Application of the Genetic Algorithm to Investigate Nanostructures of GaAs/AlGaAs Quantum Wells

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Abstract: Application of the Genetic Algorithm to the GaAs/AlGaAs quantum wells are presented. We followed a method that is produced by using the Genetic algorithm, Variation method and Monte Carlo integration Scheme (GMV method). We have investigated the effect of the well width on the diamagnetic shift. The effect of the Al doping is also investigated.

Key words: Genetic algorithm, quantum well, Monte Carlo, diamagnetic shift, method, Iran

INTRODUCTION

Genetic Algorithm (GA) inspired by the biological world is a general search and optimization method. It was first proposed by Holland in 1975. GA has been applied to many scientific areas especially in engineering optimization problems. It is also used in solving of quantum mechanical problems. In this study, we have applied this method to different realistic quantum mechanical problems of both self-consistent and non-self consistent type (Banyai and Koch, 1993). The recent developments in the fabrication technology have given an opportunity to confine the electrons in two, one and zero-dimensional semiconductor structures. Semiconductor quantum nanostructures (quantum wells, wires or dots) have found various application areas especially as electronic devices such as single electron transistor, quantum well and quantum dot infrared photo detector (QWIP and QDIP). Therefore, these structures have been intensively studied both theoretically and experimentally in condensed matter physics. Many analytical and numerical studies on energy levels and other physical properties of Quantum Dots (QDs) have been reported. Different techniques and approximations had been used in these studies including variational method, perturbation method, matrix diagonalization, Monte Carlo, etc. Each one of these techniques has their own advantages and disadvantages (Bastard, 1988). For example, the traditional variational method has the advantage of being simple and straightforward hence, it is one of the most frequently used techniques. However, the chosen trial wave function must be well suited for describing the system under consideration. If the wave function is not properly chosen, the results may be far from the exact ones. In addition to these techniques, recently, an optimization method namely the genetic algorithm has begun to be used in computations of the electronic structures (Mitchell, 1998). Genetic Algorithm (GA) has been applied to many scientific areas and engineering optimization and improvement problems since it was proposed by Holland (1975). Bennett and Shapiro have applied the GA to the ground states of simple random Ising-spin systems.

The quantum mechanical application of GA is usually called Quantum Genetic Algorithm (QGA) and is generally limited only to textbook problems. QGA involves the minimization of the total energy just like in conventional variational method but it has a probabilistic nature. When it is used in wave function optimization, the wave function in the QGA is not constrained by a prescribed analytical form and it gives results much better than conventional variational method. Application of QGA is not complicated and it can be applied to any problem stated on a variational basis. The choice of the initial population is not very important, the system under consideration need not be represented very well by the initial population. Especially, after a few tens of generations, the method converges to a wave function which quite satisfactorily describes the system under consideration (Bimberg *et al*., 1999). This fast initial convergence of the method is used in some hybrid methods for the determination of sufficiently good initial guesses. However, starting out with a population describing the system very well of course, decreases the time required for the convergence.

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Here, we have applied the method to a single quantum well GaAs/AlGaAs and extracted the diamagnetic shift as a function of magnetic field, mutation probability, population number, number of genetic iteration and upper bound of the free parameters.

MATERIALS AND METHODS

Simulation models: In spite of the fact that quantum mechanical applications of GA method is based essentially on energy minimization as other variational procedures, it exhibits some important differences. These differences can be summarized as follows:

- GA employs the coding of any parameter (or parameter set), not parameters themselves
- It starts from any initial population of possible solution, not from a single value or analytical expression
- It uses some fitness (or objective) information in procedure, not any derivative or auxiliary knowledge
- It follows the probabilistic rules, instead of the deterministic ones
- In the QGA method all the parameters can be changed simultaneously so that a faster convergence can be obtained especially for the variational problems with many parameters

The first step in this research is the old simple variational scheme exploits the ground states energy and eigenfunction of an arbitrary quantum system. In this scheme one has to select an arbitrary normalized wave-function (this selected eigen-function is better to resemble the original one) then using the following formula the ground state eigen energy can be extracted (Coley, 2001):

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

Here, in order to describe the method, we have applied the method to a symmetric quantum well to investigate the diamagnetic shift. For this purpose, we have used the Hamiltonian of the following form:

$$H = \sum_{i=e,h}\left(-\frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial z_i^2} + V_i^{conf}(z_i)\right) - \frac{\hbar^2}{2\mu}\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} - \frac{e^2}{\varepsilon_0\sqrt{\rho^2+(z_e-z_h)^2}} + \frac{1}{8}\mu\omega_c^2\rho^2 \quad (2)$$

And the trial wave function is selected as follows:

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

where, f_i $(z_{i=e,h})$ are the envelop functions and λ, a and b are the free parameters of this trial wave function that can be found using minimization of the:

$$E_0(B) = \min_{a,b,\lambda}\langle\psi|H|\psi\rangle$$

The reduced mass is $\mu = (1/m_e+(\gamma_1+\gamma_2)/m_0)$ where γ_1 and γ_2 are the Kohn-Luttinger band parameters. The diamagnetic shift is also simply defined as $\delta = E_0(B)-E_0(B = 0)$. As we know the accuracy of the variation method is strongly depend on the number of free parameters of the trial wave function but as this number grows the cpu time to determine them will also simultaneously grow. Unlike the other minimization techniques the Genetic algorithm is able to search simultaneously a large number of variables and due to the stochastic nature of this approach it is able to explore both local and global minima's at the same time. The algorithm we have used in this research is as follows: The approach is a subset of the Real Code Genetic algorithm. At first a number of descendents (the parameters we want to know them N, population) are generated. Then by using a fitness function (in this research E_0 (B) the propriety of each member of the population is evaluated. The fitness function determines that which of the members will be alive in the next iteration of the Genetic algorithm. The value of this function that can be achieved using integration is computed using a Monte Carlo scheme. The Monte Carlo method permits one to find the value of integration to a high order of accuracy by only small mesh point for the integration while the integrand is slowly varying. However, if the integrand vacillate too quickly one has to use another integration scheme instead of the Monte Carlo method. Now the members are sorted as that of their value of the fitness function. Half of them are retained with the most fitness values and the same numbers of members are produced from the first half of members that we had retained. New members are produced by using the crossover and mutation. The mutation probability plays an essential role in the results. We have shown this effect in one of the diagrams that is presented below.

The fitness values for new members are calculated. By using merge sort two different half of the population are combined in such a manner that the resulting populations are decreasingly sorted. This loop is iterated until the appropriate parameters with the desired accuracy are computed.

At first step, it seems an upper bound for the free parameters helps one to have newer members at each genetic operation and more newer ones have a chance to come to existence thus we should reach the results more rapidly (Goldberg, 1999). In other words enlarging the

interval for the free parameters lead to the results more quickly because it searches them in a larger interval but the diagrams show a different consequence.

RESULTS AND DISCUSSION

By applying the method to a single quantum well GaAs/AlGaAs we have found the diamagnetic shift as Fig. 1 for free and localized excitons. The initial parameters are the same with that used by Liu but as it can easily be seen from the Fig. 1; there are some differences in them. It has different sources. The 1st one is in the genetic algorithm. When one uses the genetic algorithm to investigate some problem it is compulsory to find the best mutation probability. Figure 2 shows the variation of the diamagnetic shift as a function of the mutation probability and the applied magnetic field in Tesla. As the Fig. 2 shows there are an oscillatory aspect versus the mutation probability thus it is not reasonable to use an arbitrary mutation probability to fine the diamagnetic shift. However, one has to find the mutation probability that lead to the least ground state energy. Other sources of errors are the number of genetic iterations at different upper limit for the free parameters when the population number is fixed Fig. 3 and 4, population number itself for a fixed number of genetic iteration, Fig. 5 and the upper limit for the free parameters, Fig. 6. It is clear from the Fig. 4 that in a fixed population number we have reached the best results when we used 1 for upper limit for the upper limit for the free parameters. As we have mentioned before, in first step, it seems an upper bound for the free parameters may help to have newer members at each genetic operation. This means new members have a chance to come to existence thus we should reach the results more rapidly. In other words enlarging the interval

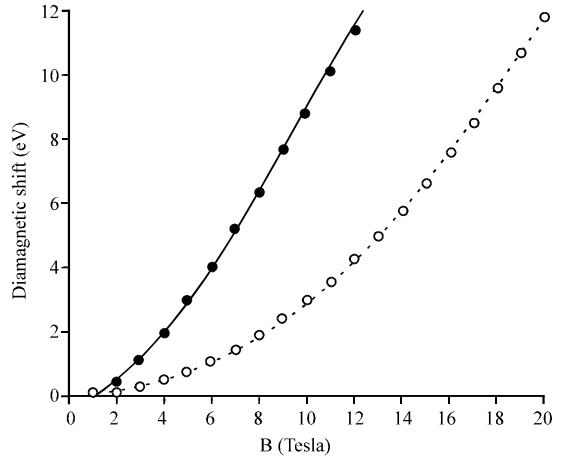

Fig. 1: Variation of the diamagnetic shift of the heavy-hole excitonic transition in a GaAs/AlGaAs quantum well with a thickness of 50 Å as a function of the magnetic field. Solid curve is calculated using the free exciton model by the method presented here and the Dashed curve is according to Liu

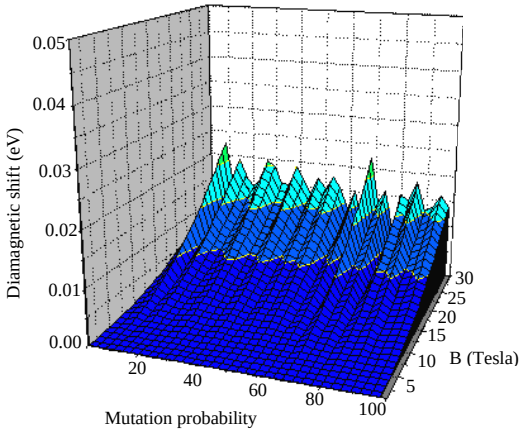

Fig. 2: Diamagnetic shift as a function of mutation probability and the applied magnetic field

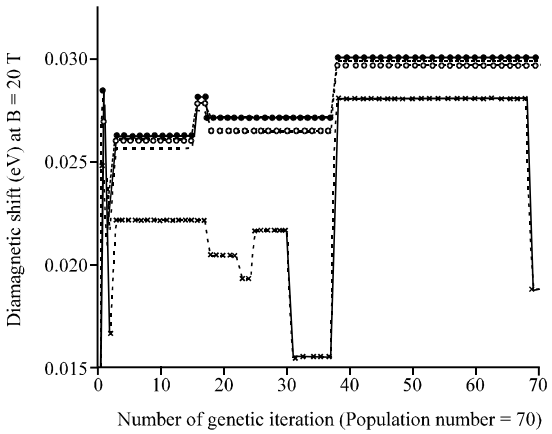

Fig. 3: Diamagnetic shift as a function of number of Genetic iteration at B = 20 T

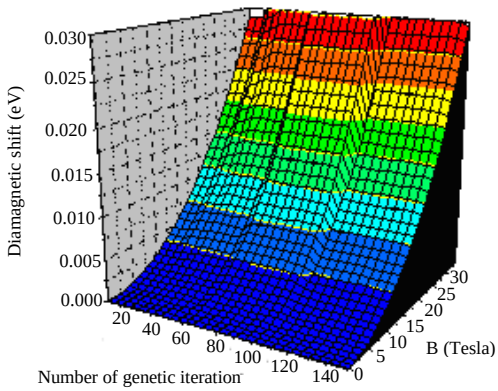

Fig. 4: Diamagnetic shift as a function of magnetic field and number of genetic iteration

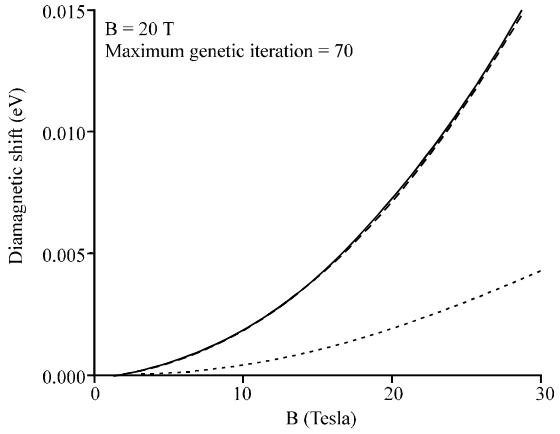

Fig: 5: Diamagnetic shift as a function of population numbers in each genetic iteration at maximum genetic iteration 70 and Bx = 20 Tesla

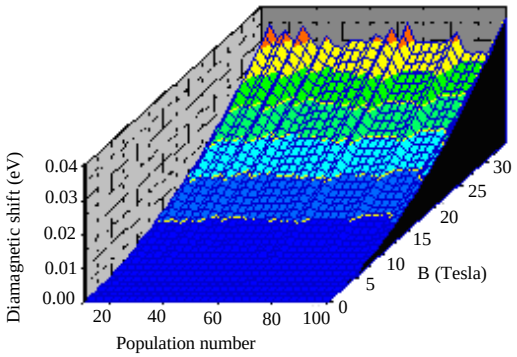

Fig. 6: Diamagnetic shift as a function of population number and magnetic field B at maximum Genetic iteration 70

for the free parameters lead to the results more quickly because it searches them in a larger interval but the diagrams show a different consequence. As Fig. 4 and 6 show when the upper bound for the free parameters is smaller the results are much better. The reason is that having a large number of choices for new member disturbs the process of finding the most appropriate one. Enlarging the interval for the free parameters gives a choice of existence to the new members and the genetic iteration searches a larger interval but when the candidate for the best parameters of the system is larger then the selecting of the best ones is also more difficult. Other reason may be random generator used in the simulation. However, before starting to extract the results it is necessary to font the optimum condition. Another result that was not so strange was that increasing in the number of genetic iteration always does not lead to a higher accuracy and only it oscillate around the real value that is shown in the Fig. 5. When the effect of changing in the population number at a fixed magnetic field B = 20 Tesla was investigated the Fig. 5 showed an oscillatory behavior. As the Fig. 5 shows the diamagnetic shift oscillates around an average value we have presented with the dashed line. Then we changed the values of the magnetic field B and extracted the Fig. 6 in a 3D plot. In both Fig. 2 and 6, the effects of the Genetic algorithm components like population number and mutation probability at low magnetic field are small but by increasing it the theses effects are more visible. In summary, we have investigated a hybrid method based on Genetic algorithm using variational and Monte Carlo sachems. For illustration purposes we have applied the method to a single quantum well and extracted the diamagnetic shift as a function of magnetic field, mutation probability, population number, number of genetic iteration and upper bound of the free parameters. It is proved that when one uses Genetic algorithm to investigate some problem, the effect of the Genetic algorithm component like mutation probability and population number may be so large that lead to wrong physical results.

CONCLUSION

Researchers have calculated the electronic structure of GaAs/AlGaAs quantum wells using the Genetic algorithm. We followed a method that is produced by using the Genetic algorithm, Variation method and Monte Carlo integration Scheme (GMV method). We have investigated the effect of the well width on the diamagnetic shift. The effect of the Al doping is also investigated.

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