Journal of Engineering and Technology Research Vol. 2(12), pp. 250-256, December 2010
Available online at http:// www.academicjournals.org/JETR
ISSN 2006-9790 ©2010 Academic Journals

Full Length Research Paper

Some new aspect of the application of Genetic algorithm to investigate nanostructures

M. Solaimani[1], M. Izadifard[1], H. Arabshahi[2]*, M. R. Sarkardehi[3] and M. Salmani[4]

[1]Faculty of Physics, Shahrood University of Technology, Shahrood, Iran.
[2]Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran.
[3]Department of Physics, Al-Zahra University, Vanak, Tehran, Iran.
[4]Department of Computer, Shahid Chamran University of Ahvaz, Ahvaz, Iran.

Accepted 17 November, 2010

Some new aspect of the application of Genetic algorithm to nanostructures is presented. We followed a method that is produced by using the Genetic Algorithm, Variation method and Monte Carlo integration Scheme (GMV method). Computational algorithm, deficiencies and advantages of the method is described and it is applied to a GaAs0.7Sb0.3/GaAs quantum well.

Key words: Genetic algorithm, variation method, Monte Carlo integration scheme, quantum well, diamagnetic shift, Pacs: 75.80. +q, 75.0.Gw.

INTRODUCTION

Anisotropy, confinement effect, quantum coherence, surface and interface effects, etc. in nanostructures, have unique properties that are not seen in bulk materials. These unique behaviors lead scientists to have great interest in them, although there are lots of difficulties in the methods of their growth. In order to have more appropriate structures with the same unique property, a vast number of theoretical and numerical approaches are produced. Finite-difference time-domain (Anderson, 1973), random walk (Zhu, 1988), genetic algorithm (Zhu et al., 1990), density matrix renormalization group (Bose et al., 1990), variation method (Varshni, 1998), perturbation approach (Huang et al., 1999), Monte Carlo method (Hai-Qing et al., 2005), power series expansion (Marin et al., 1998) and the exact solution (Ozmen et al., 2009) are some of the methods used in literatures to investigate the nanostructures.

Here, we follow a method that simulate and investigate properties of low dimensional nanostructures. The aim of this work is to combine the power of genetic algorithm for global searching, the flexibility and speed of Monte Carlo integration for multidimensional integrands and the simplicity and accuracy of the variation method to produce an optimized approach to investigate nanostructures. In this way, to some extent, we reached the mentioned goals, but just like the other computational approaches, we encountered some difficulties and deficiencies that are described in details in the foregoing and some schemes are presented in order to resolve them. The main properties of this method are its simplicity in programming, flexibility and applicability to different problems with several types of potential, simple application of boundary conditions and the power of global searching to avoid falling in the local minima. A considerable property of genetic algorithm that we have used in this work is that the genetic algorithm does not need any special approach to find the answer, but it uses some random initial answers, and in some iteration, the most appropriate one is found. When one works with problems such as quantum structures, this property simply leads to the answer; although the complexity of the type of potential may grow considerably. At last, we have applied the method to a single quantum well ($GaAs_{0.7}Sb_{0.3}$/GaAs) and have 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.

THEORY

The first step in this work is the old simple variational scheme that exploits the ground states energy and eigen function of an arbitrary quantum system. In this scheme, one has to select an arbitrary normalized wave-function (this selected eigen-function is in

*Corresponding author. E-mail: arabshahi@um.ac.ir.

resemblance of the original one), and then using the following formula, the ground state eigen energy can be extracted (Makarov et al., 2000);

$$E_0 = \min \int \psi^* H \psi dr \quad \text{..... (1)}$$

Here, in order to describe the method, we applied the method to a symmetric quantum well to investigate the diamagnetic shift. For this purpose, we have used the Hamiltonian of Senger et al. (2001), which is as follows:

$$H = \sum_{i=e,h} \left(-\frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial z_i^2} + V_i^{conf}(z_i) \right) - \frac{\hbar^2}{2\mu} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{e^2}{\varepsilon_0 \sqrt{\rho^2 + (z_e - z_h)^2}} + \frac{1}{8} \mu \omega_0^2 \rho^2 \quad \text{.....(2)}$$

In addition, the trial wave function is selected as follows:

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

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 a minimization of $E_0(B) = \min_{a,b,\lambda} \langle \psi | H | \psi \rangle$. 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 (Ren et al., 2001). The diamagnetic shift is also simply defined as $\delta = E_0(B) - E_0(B=0)$.

As it is known, the accuracy of the variation method strongly depends on the number of free parameters of the trial wave function, but as this number grows, the cpu time to determine them will also grow simultaneously. Unlike the other minimization techniques, the genetic algorithm is able to search for a large number of variables simultaneously, 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 that was used in this work is as follows. Our approach is a subset of the “real code genetic algorithm”. At first, a number of descendants (the parameters we want to know them, N, population) are generated. Then by using a fitness function (in this work $E_0(B)$) the propriety of each member of the population is evaluated. The fitness function determines which of the members will be alive in the next iteration of the genetic algorithm, while 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 a small mesh point for the integration, while the integrand slowly varies. However, if the integrand vacillates 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 the members that we had retained. New members are produced by using crossover and mutation, since mutation probability plays an essential role in the results. We have shown this effect in one of our diagrams that is thus presented. Nonetheless, the fitness values for new members are calculated. By using the merge sort, two different halves of the populations are combined in such a manner that the resulting populations are decreasingly sorted. This loop is iterated until the decreasingly sorted. This loop is iterated until the appropriate parameters with the desired accuracy are computed.

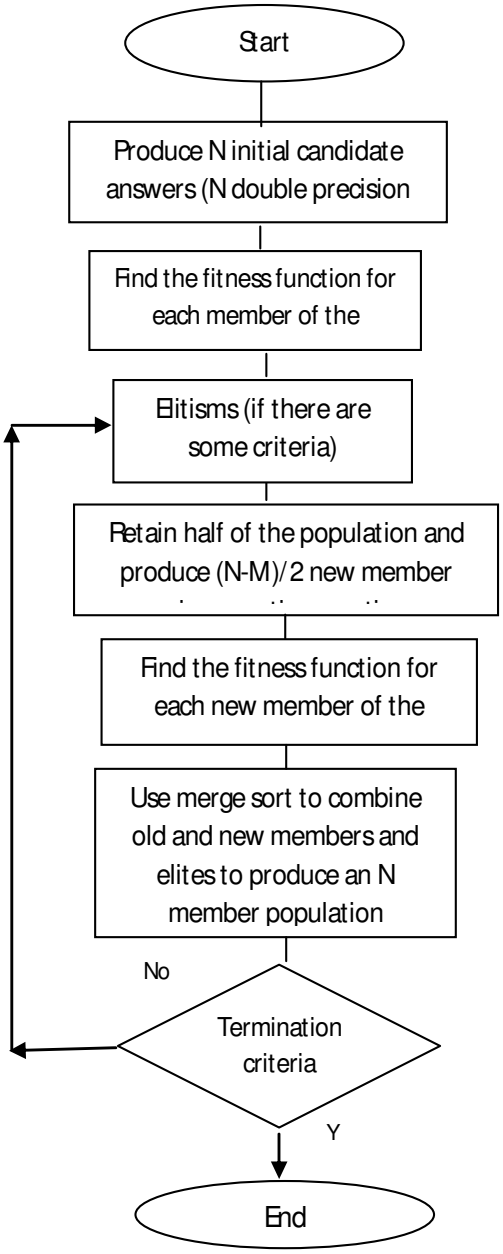

Figure 1. Flow chart of the Hybrid method we have used in this study.

At the first step, it seems that an upper bound for the free parameters helps one to have newer members at each genetic operation and more new ones have a chance to come to existence, thus the results could be reached more rapidly. 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. Hence, more information is presented in the foregoing.

At last, for the termination criteria, different schemes may be used, for example, non changing ground states energy or a predetermined number of genetic iterations. Figure 1 shows the flowchart of the study’s program.

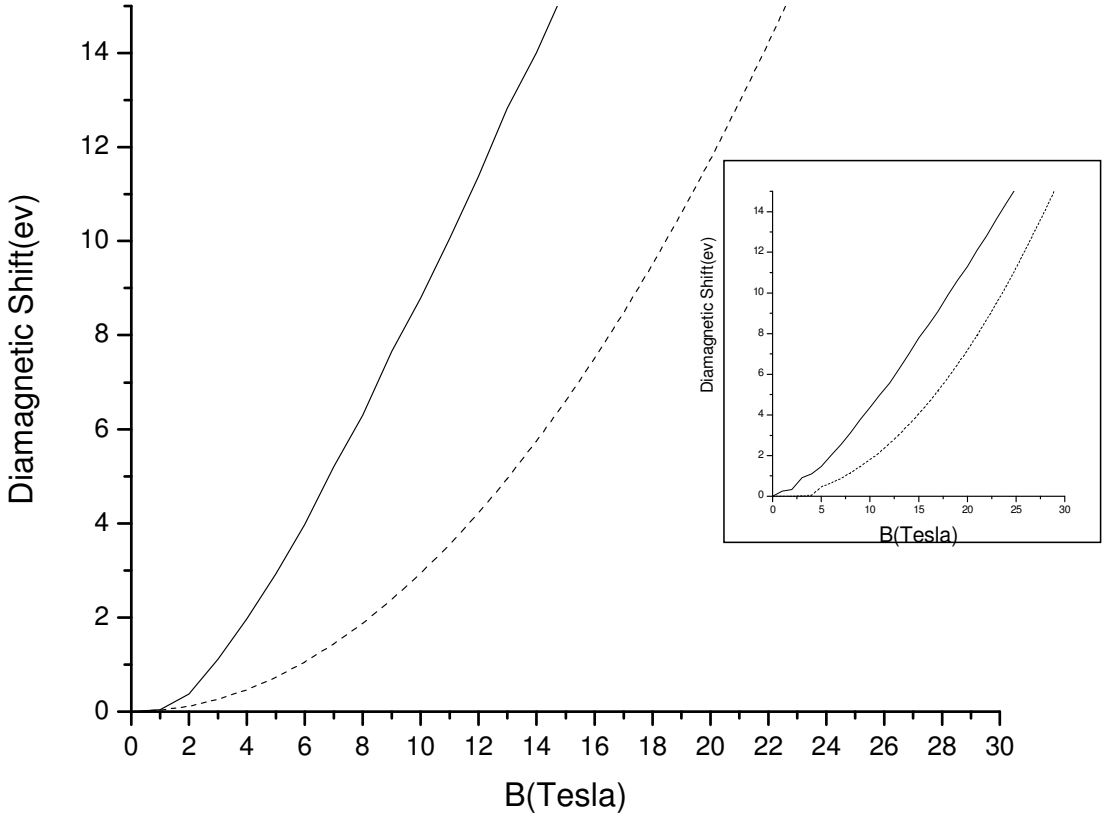

Figure 2. Variation of the diamagnetic shift of the heavy-hole excitonic transition in a GaAs0.7Sb0.3 /GaAs quantum well with a thickness of 60 angstrom as a function of the magnetic field. Solid Curve is calculated using the free exciton model by the method presented here and the Dashed Curve is according to ref 17. In both cases, the conduction-band offset ((ΔEc) is assumed to be 10 meV in a weak type-I band lineup configuration. The inset graph represents the same variation but for heavy-hole excitonic transition. Again, Solid Curve is calculated using an infinite mass for the localized heavy hole by the method presented here and the Dashed Curve is according to ref. 17 and again, in both cases, the conduction-band offset (ΔEc) is assumed to be 10 meV in a weak type-I band lineup configuration.

RESULTS AND DISCUSSION

By applying our method to a single quantum well $GaAs_{0.7}Sb_{0.3}$/GaAs, we have found the diamagnetic shift of Figure 2 for free and localized excitons. Our initial parameters are the same with that of ref 17, but as it can be easily seen from Figure 2, there are some differences in them; in that it has different sources. The first one is in the genetic algorithm. When one uses the genetic algorithm to investigate some problems, it is compulsory to find the best mutation probability. Figure 3 shows the variation of the diamagnetic shift as a function of the mutation probability and the applied magnetic field in Tesla. As Figure 3 shows an oscillatory aspect versus the mutation probability, it is, thus, not reasonable to use an arbitrary mutation probability to find the diamagnetic shift. However, one has to find the mutation probability that leads 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 (Figures 4 and 5), the population number itself is fixed for a number of genetic iteration (Figure 6) and the upper limit for the free parameters (Figure 7). It is clear from Figure 4 that in a fixed population number, the best results could be reached when "1" is used for the upper limit of the free parameters. As we have mentioned before, in the first step, it seems that an upper bound for the free parameters may help one to have new members at each genetic operation. This means new members have a chance to come into existence, thus the results could be reached more rapidly. In other words, enlarging the interval for the free parameters lead to the results more quickly because it searches for them in a larger interval, but the diagrams show a different consequence. As shown in Figures 4 and 7, when the upper bound for the free parameters is smaller, the results are much better. Consequently, the reason is that having a large number of choices for new member disturbs the process

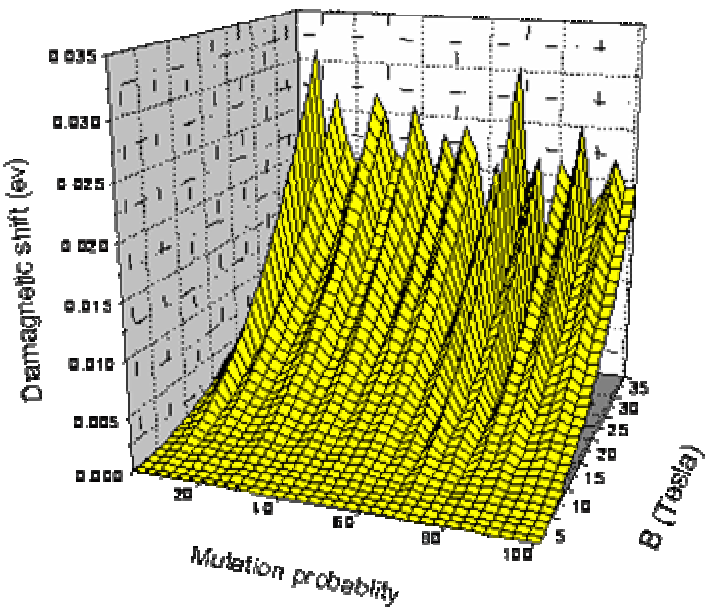

Figure 3. Diamagnetic shift as a function of mutation probability and the applied magnetic field B(in Tesla).

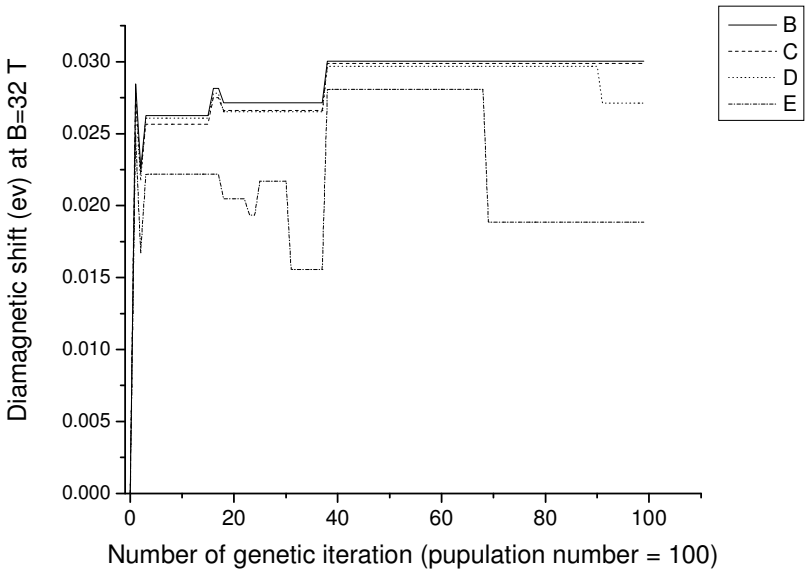

Figure 4. Diamagnetic shift as a function of number of Genetic iteration at B = 32 T population number = 100 and upper bound of the free parameters of 1,solid curve 10, Dashed Curve, 20, Dotted Curve, and 100, Dotted–Dashed curve.

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 for a larger interval; but when the candidate for the best parameters of the system is larger, the selection of the best ones is also more difficult. Other reasons may be a random generator that is used in the simulation. However, before extracting the results, it is necessary to font the optimum condition. Another result that was not so strange was the increase in the number of genetic iteration, which does not always lead to a higher accuracy, but only oscillates around the real value that is presented in Figure 5.

When the effect of changing the population number at a

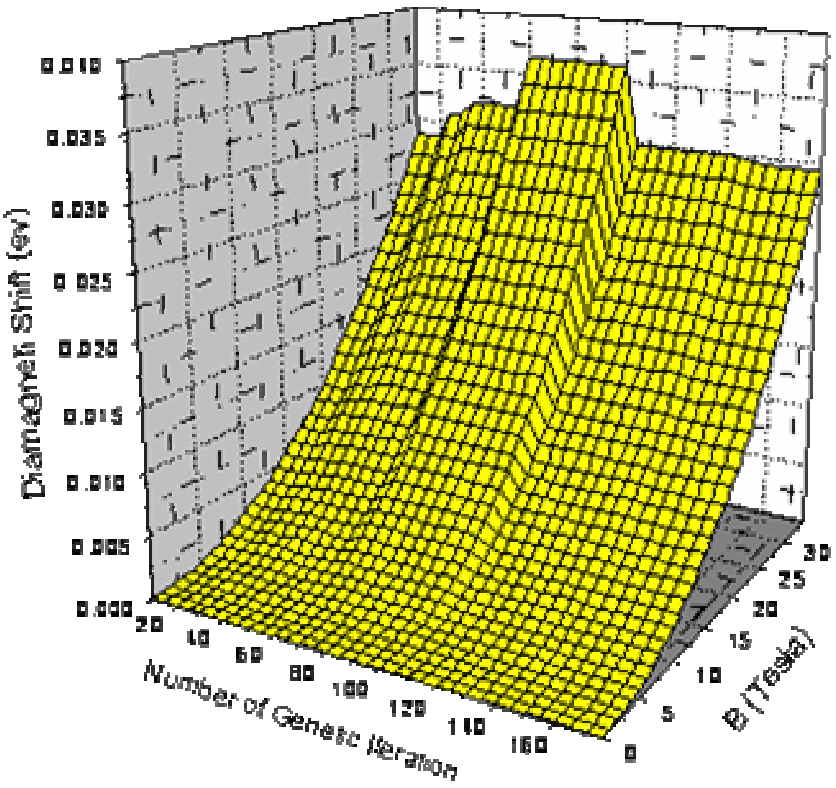

Figure 5. Diamagnetic shift as a function of magnetic field and number of genetic iteration.

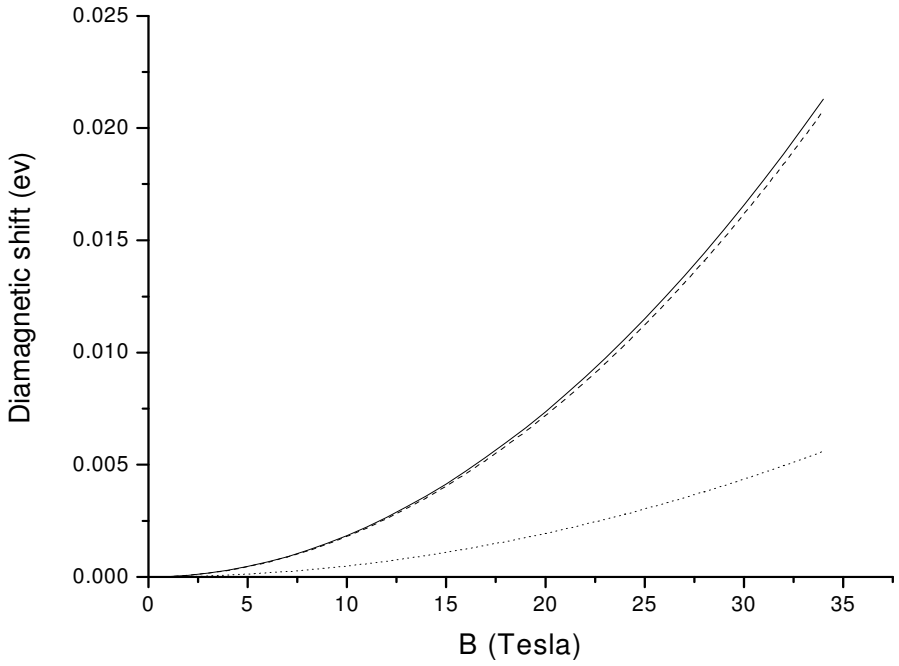

Figure 6. Diamagnetic shift as a function of population numbers in each genetic iteration at maximum Genetic iteration 100 and B = 32 Tesla.

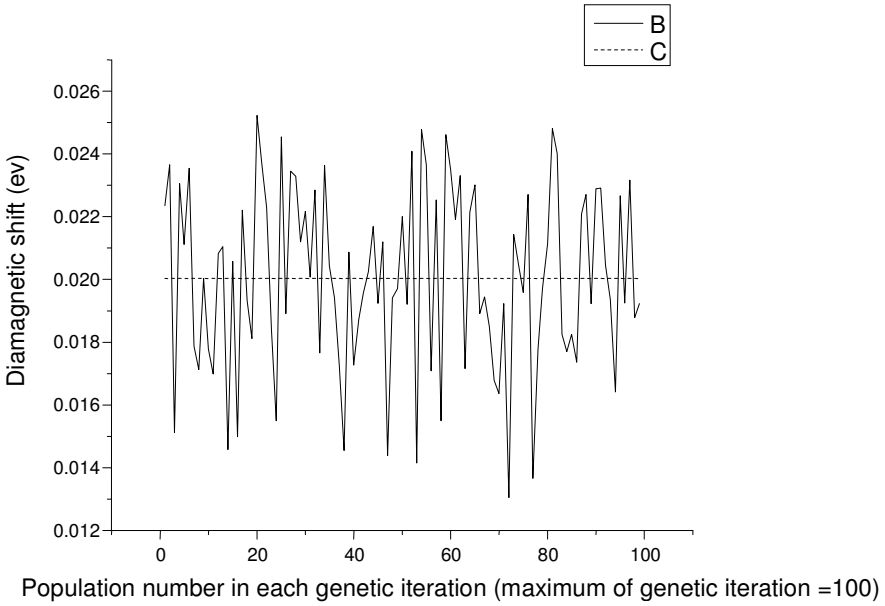

Figure 7. Diamagnetic shift as a function of upper bound of the free parameters of 1, Solid Curve, 100, Dashed Curve, and 300, Dotted.

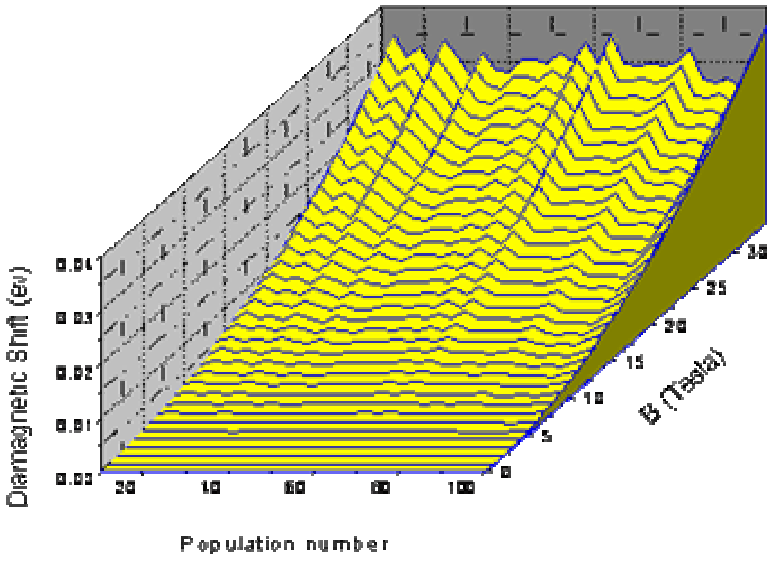

Figure 8. Diamagnetic shift as a function of population number and magnetic field B at maximum Genetic iteration 100.

fixed magnetic field B = 32 Tesla was investigated, Figure 6 showed an oscillatory behavior. Figure 6 shows that diamagnetic shift oscillates around an average value, when the dashed line was presented. Then we changed the values of the magnetic field B and extracted Figure 8 in a 3D plot.

In both Figures 3 and 8, 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 schemes. 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 has been proven that when one uses genetic algorithm

To investigate some problems, the effect of its components, like mutation probability and population number, may be so large that it will lead to wrong physical results.

ACKNOWLEDGMENT

We would like to thank Mr. Mohhamad Ali Vahedi for his beneficent conversations on the genetic algorithm.

REFERENCES

Anderson JB (1975). A comprehensive review of genetic algorithm. J. Chem. Phys., 63: 1499-1502.
Bose C, Sarkar C (1990). Systematic treatment of displacements, strains, and electric fields in density- functional perturbation theory. Physica B. 253:238-246.
Huang YS, Yang CC, Liaw S (1999). Application in genetic algorithm to the devices. Phys. Rev. A., 60: 85-92.
Hai-Qing Y, Chen T, Hao Z (2005). Hybrid method in solid state physics. Common. Theory Phys., 44: 727-732.
Marin JL, Cruz SA (1991). Population number in genetic algorithm. J. Physics B., 24:2899-2903.
Makarov DB, Metiu H (2000). Scaling down the genetic algorithm problem. J. Phys. Chem. A., 104:8540-8546.
Ozmen A, Yakar Y, Cakir B, Atav U (2009). Variational scheme in physics. Optics communications. 282:3999-3406.
Ren GB, Rorison JM (2004). Monte Carlo method in comparison to other methods. Physics Rev. E., 69:036705-036709.
Saha R, Bhattacharyya S (2004). Simulation of quantum well using Monte Carlo model. Curr. Sci., 86:10-16.
Senger RT, Bajaj KK, Jones ED, Modine NA (2003). Calculation of diamagnetic shift in AlGaN/GaN quantum well. Appl. Phys. Lett., 29:2614-2619.
Varshni Y (1998). Genetic algorithm application in quantum well. Superlattices miostruct., 23:145-152.
Zhu J (1988). Comparison of MC and GA methods in semiconductor devices. J. Phys. Rev. B., 39:8780-8785.
Zhu Xiong J, Gu BL (1990). Calculation of mutation probability using genetic algorithm. Phys. Rev. B., 41:6001-6006.