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Full Length Research Paper

Monitoring of the genetic algorithm operators in application to the $GaAs_{0.7}Sb_{0.3}$/GaAs single quantum well nanostructure

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In this work we investigated some new aspects of a recently introduced hybrid method which was a combination of Genetic algorithm, Monte Carlo integration schema and variational method. We also added some new features to the method in order to reduce the computational costs. Now we have introduced the biased Genetic Monte Carlo Variational (BGMV). With the help of different components of the method like initial physical and computational parameters we have tried to find a more trustworthy method for nanostructure investigations. It is shown that criterions like saturation of a quantity with respect to different parameters of the Genetic Algorithm like number of Genetic iterations may not lead to accurate results. CPU time of the program as a function of the number of genetic iterations for different elitist percent is depicted. Exciton binding energy of $GaAs_{0.7}Sb_{0.3}$/GaAs is obtained.

Key words: Genetic algorithm, variational method, Monte Carlo integration scheme, quantum well, exciton binding energy.

INTRODUCTION

In order to study the nanostructure systems, different theoretical approaches such as Monte Carlo (Heaedt, 1985; von der Linden, 1992; Foulkes et al., 2001), Molecular Dynamics (Xiantao and Weinan, 2005; Entel et al., 2004; Drabold and Estreicher, 2007), tight Binding (Goringey et al., 1997; Suttont et al., 1988), Genetic Algorithm (Gutowskit, 1994), Envelope Function Approximation (Burt, 1999) have previously been devised. Among these vast numbers of methods, genetic algorithm is a mechanism put in place in order to simulate the Darwinian natural selection. By introducing the evolutionary algorithms (Schwefel, 1993; Rechenberg, 1971) a new route into the mathematical solution of the optimization problems was opened and then Holland (1975) applied this method for the first time. Afterward, Goldberg introduced a better algorithm (David, 1989). Nowadays the genetic algorithm has been used in different field of studies like, engineering (Mathur and Nikam, 2009), financial affairs (Lam et al., 2009), medicine (Ecemis et al., 2008), mathematics (Yoshimoto et al., 2003), chemistry (Sandeep and Bisht, 2006) and physics. In physics the genetic algorithm has been applied for study of crystal growth (Sayle and Johnston, 2003), chaos theory (Tao et al., 2007), partition function evaluation (Grigorenko and Garcia, 2002), force field parameterization (Bukkapatnam et al., 2006), optimum materials structure (Ryan et al., 2007), powder diffraction data (Jove et al., 2001), solution of the differential equations (Burgess, 1999), simulation of semiconductor nanostructures (Dixit et al., 2008), Hamiltonian Diagonalization (Nandy et al., 2004), Schrödinger equation solution (Saha and Bhattacharyya, 2001) and applications to quantum Dot (Grigorenko et al., 2002), nanoclusters (Zhao, 2001), nanowires (Jia et al., 2006), nanoparticles (Froemming and Henkelman, 2009)

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Table 1. Material parameters for the GaAs and $Al_{0.3}Ga_{0.7}As$/GaAs.

Material	m_e	γ_1	γ_2	ε_0	Reference
GaAs	0.067	6.98	2.06	12.5	Senger et al. (2003)
$Al_{0.3}Ga_{0.7}As$	0.067	6.93	2.15	12.5	Escorcia et al. (2004), Duque et al. (2008)

and quantum wells (Rostami et al., 2008; Cakir et al., 2010).

Application of the Genetic algorithm to find best variational parameters (Hai-Qing et al., 2005) and the effect of these algorithm parameters like generation number (Nakajima and Abe, 2000; Bhaskar et al., 2000), mutation and crossover probability (Lee et al., 2000; Din and Tseng, 2002; Kumar et al., 2006; Carro-Calvo et al., 2010) of some quantities have been done several times. However, a comprehensive study of the different components of the genetic algorithm on a physical quantity has not been performed. In this work we have used our recently introduced method (Solaimani et al., 2011), Genetic-Monte-Carlo-Variational (GMV) in order to simulate a $GaAs_{0.7}Sb_{0.3}$/GaAs single quantum well. This method is a combination of the Genetic Algorithm, Monte Carlo method and the variational schema. The exciton binding energy is used as a target physical quantity in order to prove the accuracy and stability of the method. CPU time of the method is also presented to show the efficiency of this technique. The running time can be reduced through parallelization strategies as well (Zhou and Cao, 2012), but here we have tried to do it by manipulating our previous algorithm. Beside these facts, we have added some features in order to reduce the computational costs. For this purpose we have combined the previous GMV method with a deterministic walk around parameters of the trial wave function which we named the Biased GMV (BGMV).

FORMALISM

In this work we have used the Hamiltonian of the Senger et al. (2003) in the cylindrical coordinate at zero magnetic field which reads,

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

To solve the problem in the so-called variational method we have use the trial wave function:

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

where $f_i(z_{i=e,h})$ the envelope functions, e and h are indicated in the electron and hole. The reduced mass is defined by $\mu=(1/m_e+(\gamma_1+\gamma_2)/m_0)$ where γ_1 and γ_2 are the Kohn–Luttinger band parameters, which is presented in Table 1 (Senger et al., 2003). λ, a and b are the free parameters of this trial wave function that can be found by the minimization of the $E_{ex}=\min_{a,b,\lambda}\langle\psi|H|\psi\rangle$, the lateral coordinate variable is ρ = ρ_e-ρ_h.

Analytical solution of the Equation (1) is difficult because it is not separable along different degrees of freedom. Thus for most cases people try to solve it by the variational method (Bastard et al., 1982; Brum and Bastard, 1985; Lu et al., 1991; Andrey et al., 2007; Zhang et al., 2010.).

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_{ex} is the expectation value of the Hamiltonian (1), E_e and E_h are computed by using,

$$\left[\frac{E_e}{V_e}\right]^{1/2}=\cos\left[\left[\frac{m_eE_e}{2\hbar^2}\right]^{1/2}L\right],\quad\left[\frac{E_h}{V_h}\right]^{1/2}=\cos\left[\left[\frac{m_hE_h}{2\hbar^2}\right]^{1/2}L\right] \quad (3)$$

We have solved these equations by bisection method (Press et al., 2007). We used the Ben-Daniel-Duke boundary condition in order to include the effect of the effective mass mismatch in the well and barrier (Ben Daniel and Duke, 1966). We also used the Vegard law to find the effective mass of the electron and hole in the well (Singh, 1995).

The main steps of the BGMV method are given below:

(a) Use Vegard law to estimate the parameters like effective mass of the well with the doping fraction x.

(b) Find the roots of the equations: $\left[\frac{E_e}{V_e}\right]^{1/2}=\cos\left[\left\{\frac{m_eE_e}{2\hbar^2}\right\}L\right]$

$$\left[\frac{E_h}{V_h}\right]^{1/2}=\cos\left[\left\{\frac{m_{\pm}E_h}{2\hbar^2}\right\}L\right]$$

to find E_h and E_e.

(c) Find the wave vectors K_e, k_e, K_h and k_h by continuity of f_e and f_h and first derivatives at interface where, $f_e(z_e)=\begin{cases}\cos(K_ez_e), & |z_e|<L/2\\ A_ee^{-k_e|z_e|}, & |z_e|<L/2\ .\end{cases}$ and we have similar function for hole.

(d) Create an N×3 matrix for the initial population using a uniform random number generator between 0 and 1 for a, b and Lambda in the trial wave function which N is the number of members in the population.

(e) Find the $E_{ex}=\langle\psi|H|\psi\rangle$ for each member of the population using Monte Carlo integration scheme because it is flexible enough to be generalized to more dimensions and more number of degrees of freedom. Then store these values in a one

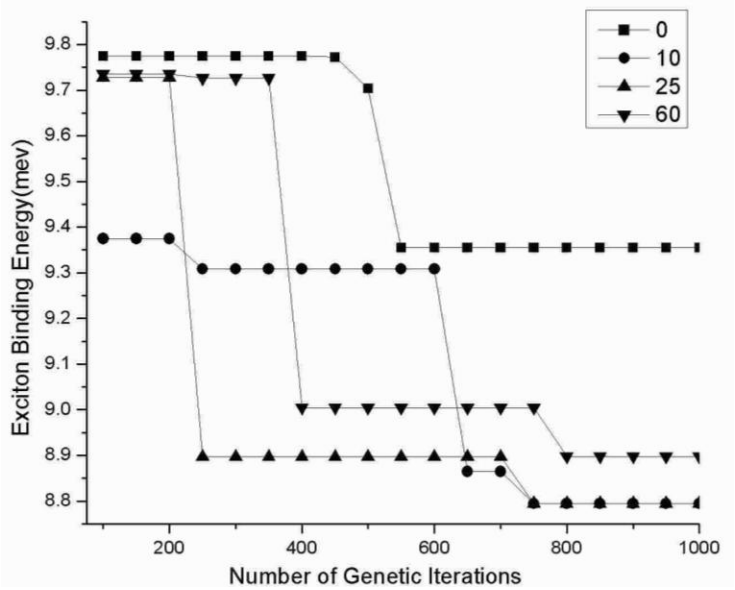

Figure 1. Variation of the exciton binding energy as a function of the number of genetic iterations for four different values, 0, 10, 25 and 60 of the 'epsilon_percent'.

dimensional array.
(f) Sort the energies obtained from previous step.
(g) Retain 'elitist' percent of lowest energies for the next generation.
(h) Generate 'epsilon_percent' of the next generation by the following method: define an infinitesimal value 'epsilon' and generate 'epsilon_percent' of the next population by adding and subtracting the 'epsilon' to the 'elitists'.
(i) Generate 'mutprob' percent of the population by the mutation.
(j) Generate the remaining number of the population by the crossover.
(k) Find the $E_{ex}=\langle\psi|H|\psi\rangle$ for new members of the population.
(l) Merge new members and old ones to have a population with relative energies in an increasing order.
(m) Go to step (g) until the termination criteria is achieved.

The new added features to produce it from the routine GMV are as follows. Firstly, we have defined a variable 'epsilon_percent' which represents a probability. By this parameter we have generated some new members in the recent population of the genetic algorithm. For this purpose we have added or subtracted an infinitesimal value 'epsilon' to the most appropriate members in the old population (that is the elitists). One may use different percent of the population as the elitist. Secondly, we have investigated the effect of the amount of this elitist number. It means that how many members in a population are elitist? The last feature is the averaging technique in order to reduce the amount of the fluctuation of a physical quantity like exciton binding energy around its true value when we plot it as a function of the number of genetic iterations.

RESULTS AND DISCUSSION

In Figure 1, the variation of the exciton binding energy as a function of the number of Genetic iterations for four different amounts of the 'epsilon_percent', 0, 10, 20 and 60 is presented. As it can be seen the values on calculated exciton binding energy is in the range in which it was previously reported (Lu et al., 1991). It is also shown in Figure 1 that 'epsilon_percent' can be used as an accuracy regulation tool in order to find the true value of the exciton binding energy. The main idea in this technique is finding the global minima and changing the best members of the population (which have the most fitness) by means of an infinitesimal value around its previous value in order to increase the accuracy. In fact when the genetic algorithm selects a point as a good answer for the problem we seek its neighboring points as probable points which may lead to a better accuracy. As the Figure 1 shows when we select a larger value for the 'epsilon_percent' we approximately get a better answer. For estimating the computational cost, CPU time versus number of genetic iteration for different values of the 'epsilon_percent' was investigated. The results which are shown in Figure 2 verify that the computational cost does not significantly change.

In order to investigate the effect of elitists' percent on the exciton binding energy its behavior as a function of the number of genetic iteration was investigated and presented in Figure 3. As the diagram shows, an increase in the value of this number reduces the energy. Our calculations were done for 1000 member populations in 1000 generations thus this diagram may be different for other values of this parameter. For example if 60% of the populations are elitists (600 members) then 400 members will be present in the procedure of the genetic algorithm. Thus in 1000 generations we may have good accuracy. In order to show the effect the elitists percent

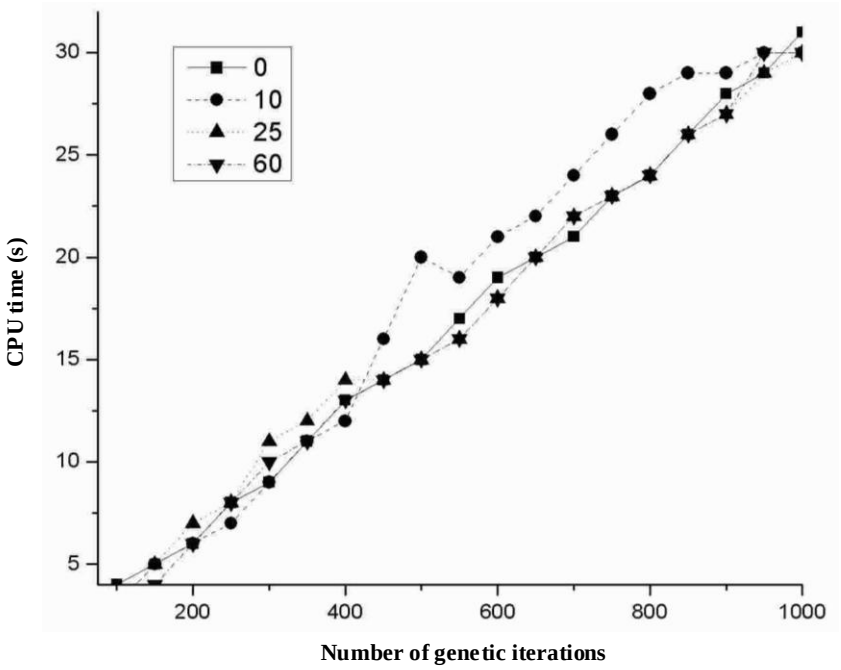

Figure 2. CPU time of the method as a function of the number of genetic iterations for four different values, 0, 10, 25 and 60 of the 'epsilon_percent'.

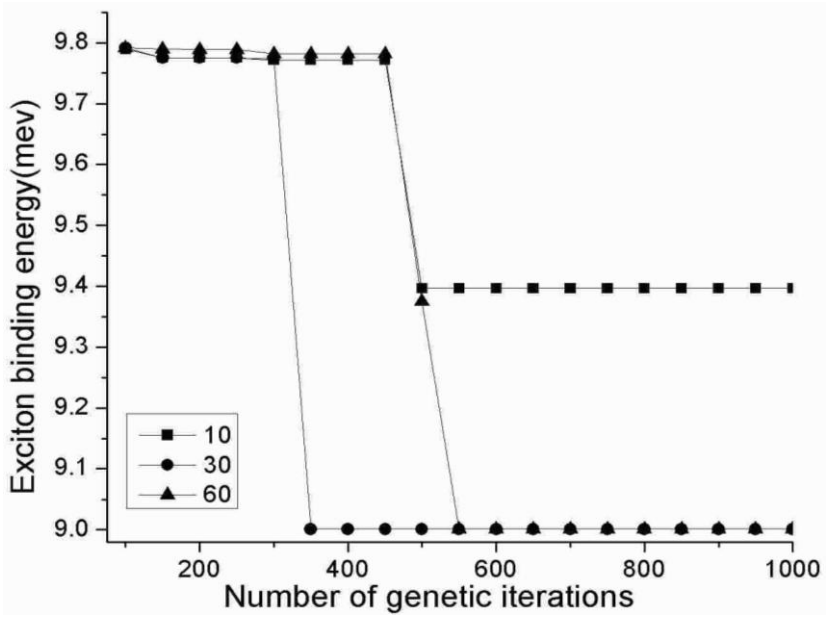

Figure 3. Variation of the exciton binding energy as a function of the number of genetic iterations for four different values, 10, 30, 60 and 90 of elitists percent.

has on the computational cost, the variation of the CPU time as function of the genetic iteration numbers for different values of elitist percent (10, 30, 60 and 90) are monitored in Figure 4. As one can see for a larger value of the elitist percent, the CPU time reduces because the number of the members in the procedure of the genetic algorithm reduces.

In Figure 5, we have presented the variation of the exciton binding energy as a function of the averaging number. The initial parameters are presented in Table 2.

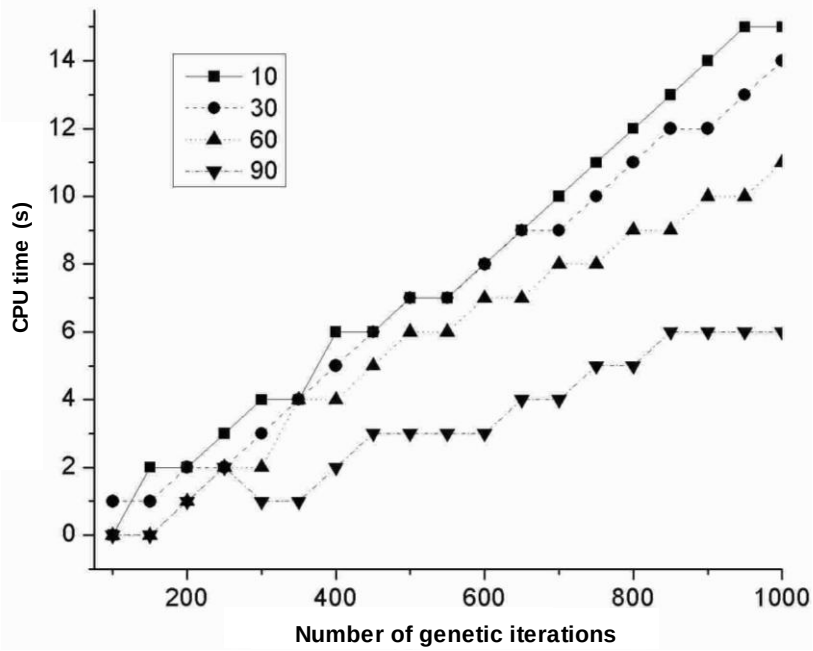

Figure 4. CPU time of the method as a function of the number of genetic iterations for four different values, 10, 30, 60 and 90 of elitists percent.

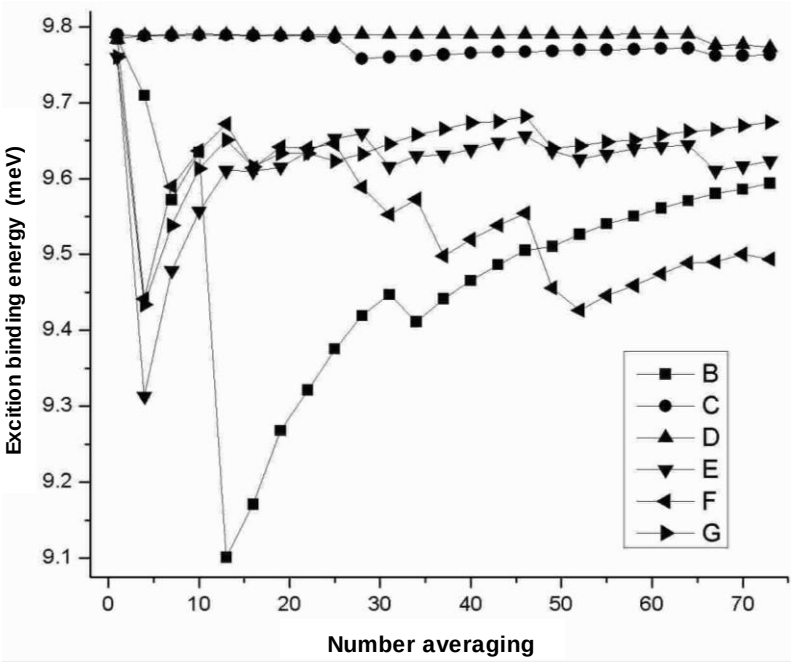

Figure 5. Variation of the exciton binding energy as a function of the number of the number of averaging. Descriptions are presented in the text.

In order to show the effect of the averaging on a physical reduce the Generations and Monte_sampling_point_number the averaging effect is negligible. This fact shows that since the envelope functions are slowly varying function thus with a small quantity like exciting binding energy we have changed different parts of these parameters and plotted them in other parts of Figure 5. As it can be clearly seen when we

Table 2. Initial parameters for different parts of the Figure 6.

Parameter	Generation	MC sampling point number	Population number	Mutation probability	Elitists percent	Epsolion percent
B	1000	700	1000	40	10	0
C	1000	700	500	40	10	0
D	500	700	1000	40	10	0
E	1000	450	1000	40	10	0
F	1000	700	1000	5	10	0
G	1000	700	1000	40	10	40

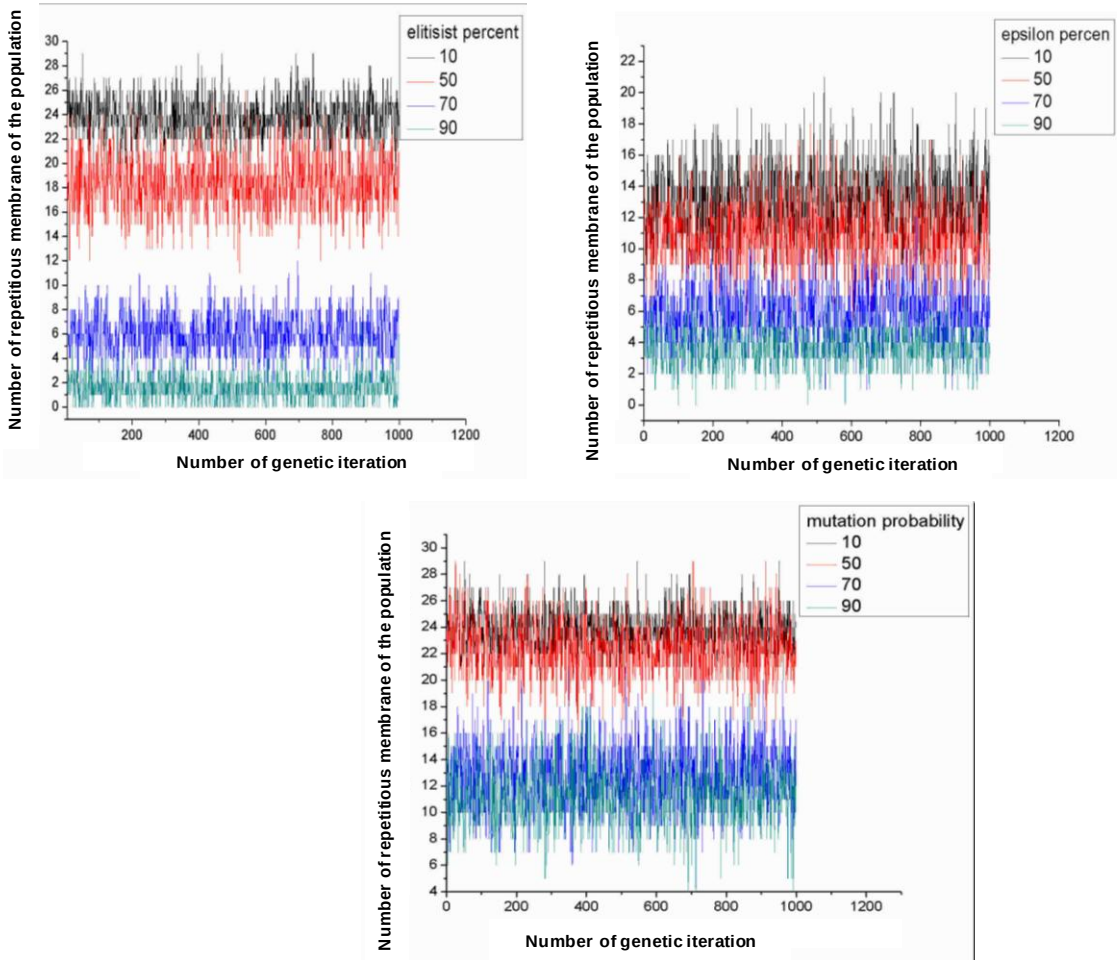

Figure 6. Variation of the number of the repetitious members in the population as a function of the number of genetic iterations by changing the 'elitists_percent', 'epsilon_percent', and the value of the mutation probability.

number of the Monte Carlo sampling points we may achieve better accuracy. The effect of averaging on the Mutation_probability and 'epsilon_percent' for small number of the averaging is large. When we increase the number of averaging their fluctuations reduce. The most fluctuations can be seen in B and F cases. Maximum effect of the averaging on the exciton binding energy is about 0.7 mev.

At last the numbers of the repetitious members in the population with changing the values of the previously discussed parameters like epsilon_percent, Mutation_probability and elitisist_percent are investigated and the results are shown in Figure 6. As we can see in this figure, for all cases when the value of these parameters increase the repetitious members decrease. In addition, when the number of genetic iterations

increases the number of repetitious members of the population oscillates around a constant value. When we increase the number of elitists the number of members in the genetic procedure reduces and thus the number of the repetitious member correspondingly is reduced. When the 'epsilon_percent' increases the repetitious numbers of members reduce because we have deterministically produced different members by adding or subtracting an infinitesimal value to some old members. Finally since we have produced new members by random changing of old members (from large to small or vice versa) and since our random generator, ran2 has a period of repetition of about 2×10^{18} (Press et al., 2007), thus when the value of the mutation probability increases the number of the repetitious member decreases. The number of the repetitious members is obtained by direct counting. Our technique helps to find the optimum initial parameters with a predetermined computational cost. Another fact is that since in our work each member has consisted of only 3 part (a, b, Lambda) therefore the repetitious members may be encountered in a large portion. However, for different situations with different number of parts in each member or in other physical situations we may see other results.

It is clear from the Figures 1 and 2, that criterion like saturation of a quantity with respect to a parameter like number of Genetic iterations which is usually used as a termination criterion may not work correctly. As we see in the Figures 1 and 2 the diagrams are saturated in different levels. Now a physical principle may help to find the best initial parameters. This means that for solving these problems with a stochastic method like genetic algorithm we have to determine the effect of the initial parameters in order to find the physical quantities. This may be done by changing the initial parameters such as mutation probability or plotting the quantity as a function of mutation probability, generations or other computational parameters.

Conclusion

In this work, we have introduced a new modified version of our previously introduced GMV method (Solaimani et al., 2011), by adding some new deterministic computational parameters like 'epsilon_percent' in order to increase the convergence rate and reduce the computational costs which the results is presented in the diagrams of the CPU times. We have added a parameter 'epsilon_percent' to the Previous GMV method which can be used as an accuracy regulation tool in order to find the true value of the exciton binding energy. As the Figure 1 shows, when we select a larger value for the 'epsilon_percent' we approximately get a better answer. By using the technique of averaging, its effect on the Genetic parameters such as Mutation_probability and 'epsilon_percent' are investigated. When we increase the number of averaging their fluctuations reduce. The most fluctuations can be seen in B and F cases of Figure 5. Maximum effect of the averaging on the exciton binding energy is about 0.7 mev. Finally, the number of the repetitious members in the population is obtained by direct counting which helps to find the optimum initial parameters with a predetermined computational cost.

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