

Full Length Research Paper

Genetic algorithm based diamagnetic shift investigations of the GaAs_{0.7}Sb_{0.3}/GaAs and Al_{0.3}Ga_{0.7}As quantum wells

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In this work we have presented some other aspects of the recently introduced GMV method (Genetic Monte Carlo Variational method). The CPU time of the method is computed and then we have applied the method to As_{0.7}Sb_{0.3}/GaAs quantum well to investigate the effect of the well width and Sb fraction on the diamagnetic shift. The effect of the Al doping instead of the Sb is also investigated.

Key words: Genetic, Monte Carlo Variational method, quantum well, Pacs: 75.80.+q, 75.0.Gw.

INTRODUCTION

Exciton behaviors under an external magnetic field (exciton diamagnetic shift) in two dimensional quantum well systems have attracted considerable interests (Crow et al., 1999) In order to evaluate the diamagnetic shift of the system, one has to solve the Schrödinger equation for a specified exciton (Escorcia et al., 2004). There are different methods that have applied to two dimensional quantum well systems (single or many particle solution methods) such as asymptotic iteration method (Zhu et al., 1987), Hartree-Fock theory (Wei, 1989), k-p theory (Boykin et al., 2002), Monte Carlo simulation (Duque et al., 2008), power series expansion (Fu et al., 2006), tight binding (Greene et al., 1984), variational methods etc. Although there are different solution methods in this field of study but existence of a simple and efficient method that has good flexibility to be manipulated may help a lot to have more reliable results. In our previous work (Juri et al., 2005) we have investigated a new hybrid method combining the Genetic Algorithm (GA), variational method and Monte Carlo integration scheme to find a reliable method in the nanostructure applications. In that work we presented the computational algorithm including the flowchart and the effect of the various genetic parameters such as mutation probability, number of

genetic iterations in the procedure of the solution of the Schrödinger equation (Lin, 1989). It was shown that the genetic algorithm procedure may affect on the physical properties (Mann et al., 1984).

Now, in this work, the CPU time of the method to finding the best variational parameters with the genetic algorithm is presented. The effects of the well width and the Sb fraction on the diamagnetic shift in As_{0.7}Sb_{0.3}/GaAs quantum well are calculated. The effect of the Al doping instead of the Sb is also investigated.

THEORY

We have used the Hamiltonian of the same as Soylu et al. (2008) which is,

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

In our variational scheme to exploits the ground states energy and eigenfunction of the system a trial wave function is selected which is as follows,

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

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

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

Material	m_e	γ_1	γ_2	ϵ_0	V_e (meV)
GaAs	0.067	6.98	2.06	12.5	50
GaSb	0.042	13.4	4.7	15.7	
Al _{0.3} Ga _{0.7} As	0.067	6.93	2.15	12.5	10.7

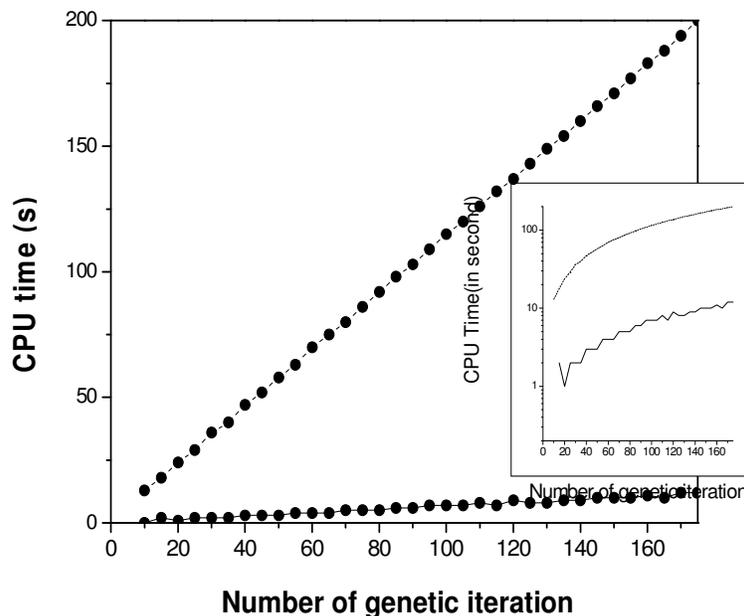


Figure 1. The CPU time as a function of the number of genetic iterations in the calculation of the diamagnetic shift. Inset, the CPU time as a function number of genetic iteration in the calculation of the diamagnetic shift in log-scale with a smaller range in the CPU time axis. The inset diagram shows that the increase in the CPU time is not completely linear. In both diagrams the solid lines is for one time run and the dashed line for 50 times run of the program.

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 (Oettinger et al., 1985). Material parameters used in this work are presented in the Table 1 (Hilton et al., 1992). The diamagnetic shift is also simply defined as $\delta = E_0(B) - E_0(B=0)$.

RESULTS AND DISCUSSION

One of the most important features in a computational method is the CPU time. It shows the flexibility of the method and determines its power to reach the solution. We have plotted the CPU time of the GMV method as a function of the genetic iterations numbers in the Figure 1. As it can be seen the CPU time grows linearly with

number of genetic iterations. To be clearer we have plotted the CPU time in a log-scale but in a smaller range in the CPU time axis. It shows that its growth behaves a little nonlinearly. In Figure 1 and its inset, the solid lines is for one time run and the dashed line for 50 times run of the program. In some applications one has to run the program several times, each time with a bit of change in some variable (magnetic field for diamagnetic shift calculations in this work), thus we have tested the CPU time for the several times running of the program to test the speed.

To illustrate the effect of the well width, variation of the diamagnetic shift of the As_{0.7}Sb_{0.3}/GaAs single quantum well for $x = 0.3$ as a function of magnetic field B and the well width L in a 3-dimensional diagram is presented in Figure 2. By increasing in the well width for another Sb fraction $x = 0.7$. Figures 2 and 3 reveal the slop of the

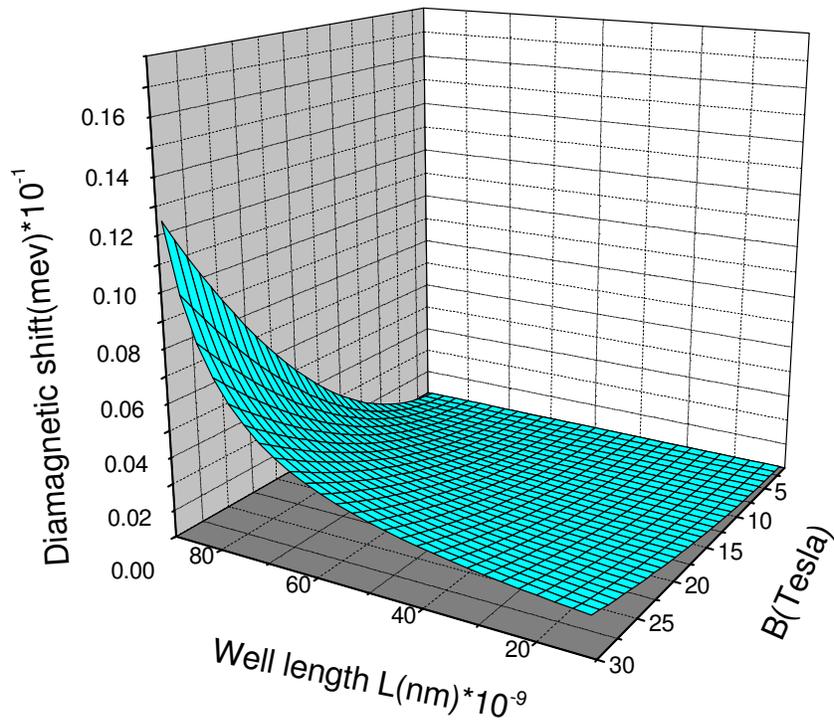


Figure 2. Variation of the diamagnetic shift for GaAs_{0.7}Sb_{0.3}/GaAs as a function of B and L for x = 0.3.

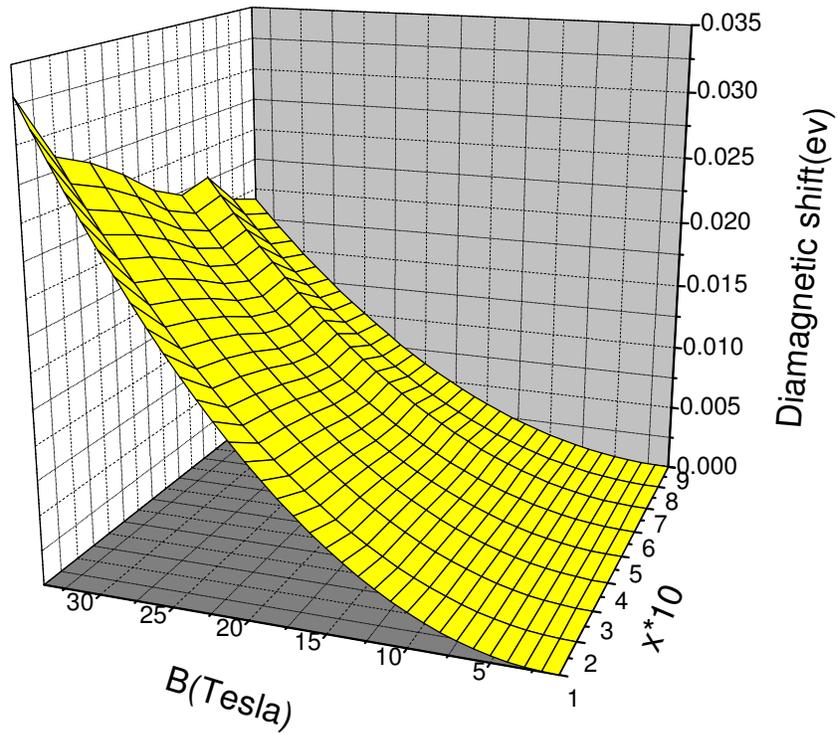


Figure 3. Variation of the diamagnetic shift for GaAs_{0.7}Sb_{0.3}/GaAs as a function of B and L for x = 0.7.

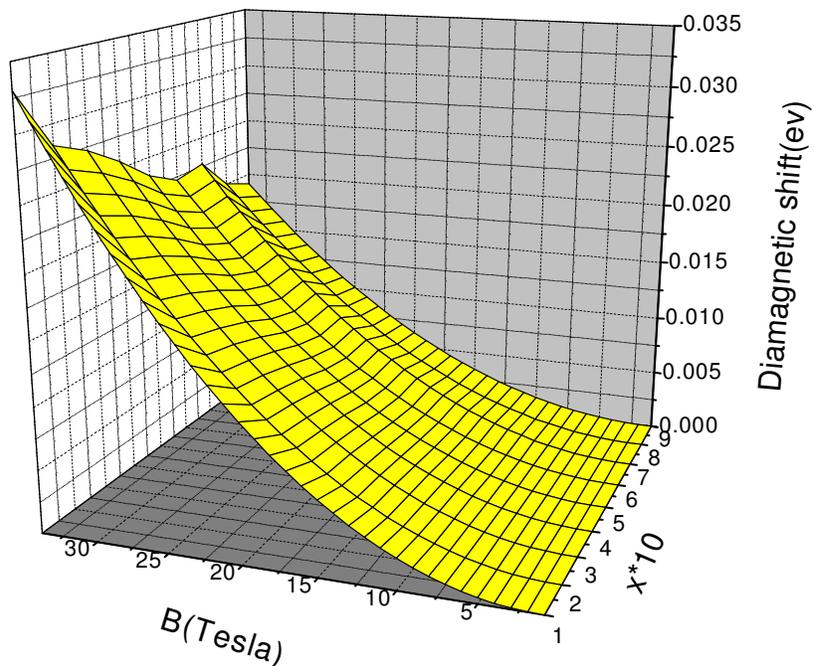


Figure 4. Variation of the diamagnetic shift for GaAs_{0.7}Sb_{0.3}/GaAs as a function B and x for the well width L = 60Å.

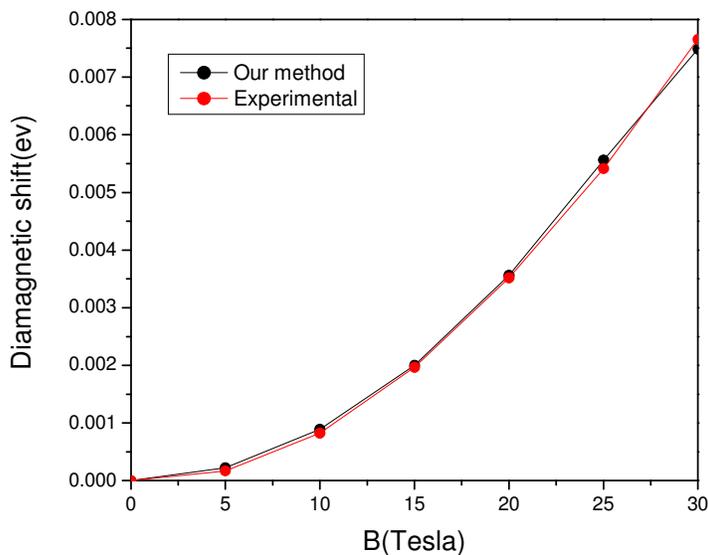


Figure 5. Variation of the diamagnetic shift for Al_{0.3}Ga_{0.7}As/GaAs as a function B for the well width L=100 Å. Red line is the experimental diagram and the black line is obtained by using our method. Extreme accordance to the experimental diagram is sensibly visible.

slop of the diamagnetic shift grows sharper. For comparison purposes we have repeated the Figure 2 that by increasing in the x-fraction the maximum values of the diamagnetic shift become smaller. This can be more understood from the Figure 4 that shows the variation of

the diamagnetic shift as a function of the magnetic field B and fraction x for a well width L = 60 Å.

We have also found the diamagnetic shift for Al_{0.3}Ga_{0.7}As that can be seen in the Figure 5 for well width of 100 Å to check the effect of the different doping.

Red line is the experimental diagram taken from reference 21 and the black line is obtained by using our method that is in extreme accordance with the experimental one and it shows the validity of our approach. It is clearly seen that the corresponding values of the diamagnetic shift for $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ quantum well is smaller than that of the $\text{GaAs}_{0.7}\text{Sb}_{0.3}/\text{GaAs}$ quantum well.

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