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QUANTUM SIMULATIONS OF SMALL ELECTRON-HOLE COMPLEXES*

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ABSTRACT

The Green's Function Monte Carlo method is applied to the calculation of the binding energies of electron-hole complexes in semiconductors. The quantum simulation method allows the unambiguous determination of the ground state energy and the effects of band anisotropy on the binding energy.

INTRODUCTION

The interaction of electrons and holes in a semiconductor is apparently well described, but not exactly described, by the effective mass Hamiltonian. This simple Hamiltonian, which has a sound theoretic basis [1], says that electrons and holes interact via a coulomb potential which is screened by the dielectric constant. The fact that electrons in the conduction band and holes in the valence band interact with a sea of other electrons and a periodic lattice of atomic cores is contained in an effective mass m_e or m_h for the electrons and holes.

$$H = \Sigma - \frac{\hbar^2}{2m_e} \nabla^2_e - \frac{\hbar^2}{2m_h} \nabla^2_h + \Sigma \frac{e^2}{K r_{eh}} \qquad (1)$$

With this Hamiltonian the study of small complexes becomes a few-body problem instead of a many-body problem. The simplest complex, the exciton, is equivalent then to a hydrogen atom and is an analytically soluble two-body problem. The existence of excitons is well known [2] from the luminesence spectra of semiconductors [3] and provide valuable information about the materials properties of semiconductors.

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Small electron-hole complexes with two holes and one electron, the trion, with two holes and two electrons, the biexciton, and larger conglomerations have been the subject of theoretical consideration [4] with supporting experimental [5] evidence for some time. These few-body problems cannot be solved analytically, and the absence of an accurate ground state energy inhibits the unambiguous identification of their contribution to the spectra from these semiconductors.

It is the primary value of quantum simulation methods that they yield accurate, indeed exact, information about quantum many-body systems. This work describes the application of the Green's Function Monte Carlo (GFMC) method to the calculation of the ground state energy of these few-body electron-hole complexes. As will be explained in the next section, the method yields the exact (or as accurate a value as desired) ground state energy, but does not give an analytic expression for the wave function. All the information one obtains about the wave function comes in the form of a set of points in configuration space sampled from a probability distribution which is proportional to the wave function.

THE GFMC METHOD

It has been appreciated for some time [6] that the mathematical structure of the Schroedinger equation is directly analogous to a diffusion equation in the presence of absorption processes. Kalos and co-workers [7] have taken this analogy and shown that it may be made into a computationally feasible method for obtaining exact information about the ground state energy and structure of quantum many-particle systems. To date, these methods and similar quantum simulation methods have been successfully applied to many-boson systems such as liquid and solid ^{4}He [8], one dimensional fermion models [9], few nucleon models [10] and lattice gauge theories [22]. Although no exact method exists [10] for simulating three dimensional many-fermion systems, considerable progress in this direction has been made for the electron gas [11], liquid ^{3}He [12], and atomic and molecular electronic structure calculations [13].

In this paper we will describe the Green's Function Monte Carlo method and apply it to the study of the four-particle (biexciton) system. Because this system has two electrons of opposite spin, and two holes of opposite spin, the antisymmetry requirement of fermion statistics does explicitly enter the calculation, and normal boson methods apply.

The Diffusion Analogy

The Schrodinger equation for an N-particle system is

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + V(\vec{r}_1, \ldots, \vec{r}_N)\right]\psi = i\hbar\frac{\partial}{\partial t}\psi. \qquad (2)$$

It will be convenient to use a 3-N dimensional vector, $R = (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$, to specify the particle positions. To avoid confusion we will restrict the term particle to refer to the three dimensional entities in real space. In 3N dimensions the position vector R will specify a configuration. With this notation, and understanding that ∇^2 is the 3-N dimensional Laplacian, the Schroedinger equation becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(R,t) + V(R)\,\psi(R,t) = i\hbar\frac{\partial}{\partial t}\psi(R,t). \qquad (3)$$

In the same notation, we wish to describe the diffusion process in 3-N dimensions. A density, $\rho(R,t)$, (to be thought of as the density of configurations having the coordinate R) gives rise to a diffusion current

$$\vec{J}(R,t) = -D\vec{\nabla}\rho(R,t) \tag{4}$$

where D is the diffusion constant. If current is not conserved, then a source term modifies the conservation equation,

$$\vec{\nabla}\cdot\vec{J}(R,t) + \frac{\partial}{\partial t}\rho(R,t) = S(R,t). \tag{5}$$

S(R,t) is the number of configurations per unit volume and time which are produced at point R. If S(R,t) is negative then its magnitude is the rate of absorption of particles. If there is a probability per unit time, A(R), for a particle at R to be absorbed, then the source term is of the form,

$$S(R,t) = -A(R)\,\rho(R,t). \tag{6}$$

Combining these three relations yields the diffusion equation in the presence of absorption.

$$-D\,\nabla^2\rho(R,t) + A(R)\,\rho(R,t) = -\frac{\partial}{\partial t}\rho(R,t). \tag{7}$$

It is the similarity of this equation to the Schroedinger equation which forms the basis of the GFMC method. In the appropriate units, ($\hbar$=1) the identifications of D with 1/2m and A(R) with V(R) make the two equations identical except for the factor $i = \sqrt{-1}$ associated with the time variable. This near equivalence can be seen clearly if at t=0 the starting point for the time evolution of both equations is the same, i.e. $\rho(R,0) = \psi(R,0)$, then the formal solution to the equations in terms of the stationary state solutions (ϕ_n) is

$$\begin{aligned}\rho(R,t) &= \sum_n a_n\phi_n(R)e^{-\lambda_n t}\\ \psi(R,t) &= \sum_n a_n\phi_n(R)e^{-iE_n t}\end{aligned} \tag{8}$$

The eigenvalues are identical $\lambda_n = E_n$ and the eigenfunctions are identical. The difference is that ψ oscillates in time and ρ decays in time. Actually, the decay process occurs only if the eigenvalue spectrum is positive definite, but this can always be achieved by subtracting a constant E_T from the Hamiltonian. This amounts to guessing a trial value for the ground state energy. At large times, the dominate component in the density is the one with the smallest eigenvalue. If one has chosen E_T to be near E_0, then asymptotically

$$\rho(R,t) \sim a_0\phi_0(R)e^{-(E_0-E_T)t} \tag{9}$$

the density is nearly time independent and converges to the ground state wave function.

The crux of the GFMC method is that it doesn't attempt to simulate the Schroedinger equation directly, but actually implements a diffusion process that evolves in time until the density approaches the ground state wave function. Equivalently, one may say that the GFMC method simulates the quantum system in imaginary time. Following the second point of view, we define the variable $\tau=it$, then Schroedinger's equation

$$(-\nabla^2 + V(R) - E_T)\,\psi(R,\tau) = -\frac{\partial}{\partial\tau}\psi(R,\tau) \tag{10}$$

has the formal solution

$$\psi(R,\tau) = \sum_n a_n\phi_n(R)e^{-(E_n-E_T)\tau}. \tag{11}$$

The Green's Function

The operator which moves the system forward in imaginary time is the Green's function,

$$G = e^{-(H-E_T)\tau}. \tag{12}$$

In terms of position space variables, the propagation of ψ is achieved by the integral

$$\psi(R,\tau) = \int G(R,\tau,R',\tau')\,\psi(R',\tau')dR'. \tag{13}$$

It is this integral which is to be done using Monte Carlo techniques.

The properties of this Green's function are contained in elementary quantum mechanics and mathematical physics texts [14]. It is only necessary to make the substitution $\tau=it$ for the purpose at hand. G satisfies a diffusion equation

$$[-\nabla^2_R + V(R)]\,G(R,\tau,R',\tau') = -\frac{\partial}{\partial\tau}G(R,\tau,R',\tau') \tag{14}$$

with the boundary condition

$$\lim_{\tau\to\tau'^+} G(R,\tau,R',\tau') = \delta^{3N}(R-R'). \tag{15}$$

It has the formal solution

$$G = \Sigma\, \phi_n(R) e^{-E_n \tau} \phi_n(R') e^{+E_n \tau'} \tag{16}$$

and can itself be propagated forward in time

$$G(R,\tau,R'',\tau'') = \int dR'\; G(R,\tau,R',\tau')\; G(R',\tau',R'',\tau''). \tag{17}$$

In the language of a diffusion process, $G(R,\tau,R',\tau')$ is the density resulting from a unit source, or equivalently, the expected density at position R at time τ given that initially one configuration was at position R' at time τ'.

One does not need an analytic expression for the Green's function in order to propagate the wave function forward in time. It is useful, however, to begin with an analytic form which is valid for short times $\Delta\tau = \tau - \tau' \ll 1$. The configuration initially at R' remains localized there for short times. For sufficiently short times the local potential may be considered to be a constant, $u = V(R')$. The Green's function for a constant potential satisfies,

$$(-\nabla^2 + u)\; G_u(R,\tau,R',\tau') = -\frac{\partial}{\partial\tau} G_u(R,\tau,R',\tau')$$

and is given by a gaussian,

$$G_u(R,\Delta\tau,R',0) = \frac{\exp\{-(R-R')^2/2\Delta\tau - u\Delta\tau\}}{(2\pi\Delta\tau)^{3N/2}}. \tag{18}$$

In terms of V(R'), including now the constant E_T added to H, G is approximately given by

$$G(R,\tau'+\Delta\tau,R',\tau') \cong \frac{\exp\{-(R-R')^2/2\Delta\tau - (V(R')-E_T)\Delta\tau\}}{(2\pi\Delta\tau)^{3N/2}}. \tag{19}$$

and neglects terms of order $\Delta\tau$ compared to unity.

At this point one can implement the GFMC method within the short time approximation. We will come back to considerations of efficiency and accuracy after outlining the short-time algorithm.

The GFMC method will not give an analytic form for $\psi(R,\tau)$, but rather supplies a set of configuration points {R} sampled from $\psi(R,\tau)$. That is to say the probability of a particular R occurring in a population of many configurations is proportional to the value of the wave function at that point. For the systems of interest here, the ground state wave function is positive definite, hence one can define the probability density

$$P(R,\tau) = \psi(R,\tau)/\int \psi(R,\tau)\, dR \tag{20}$$

and say that one obtains a set of configurations sampled from $P(R,\tau)$. Note that the probability density is in terms of the wave function and not its square.

The algorithm proceeds as follows. Initially one selects a large number ($M \sim 10^3$) of configurations $\{R_i(\tau=0)\}_{i=1}^{M}$ from some initial guess for the ground state wave function. This initial guess is usually an analytic trial wave function $\psi_T(R)$, and the initial sample can be generated using standard Metropolis techniques [15]. Given this sample for $\psi(R,0)$ one wishes to obtain configurations sampled from $\psi(R,\Delta\tau)$. The expected value of the wave function $\psi(R,\Delta\tau)$ at each point R is given by substituting the configurations $\{R_i(0)\}_{i=1}^{M}$ into equation 13. Then

$$\langle\psi(R,\Delta\tau)\rangle = \frac{1}{M}\sum_{i=1}^{M} G(R,\Delta\tau,R_i(0),0). \tag{21}$$

If one samples a new set of L points $\{R_i(\Delta\tau)\}_{i=1}^{L}$ from the probability distribution

$$\langle\psi(R,\Delta\tau)\rangle/\int dR\langle\psi(R,\Delta\tau)\rangle, \tag{22}$$

then this new set will be sampled from $P(R,\Delta\tau)$, i.e. the wave function at time $\tau = \Delta\tau$. Once complete, the process is repeated from the set $\{R(\Delta\tau)\}$ to obtain $\{R(2\Delta\tau)\}$ and integrated to arbitrarily large τ.

The simulation proceeds by allowing each of the initial configurations to diffuse for a time $\Delta\tau$. In the short time approximation G is known, and one simply sample a new set of configurations from the gaussians centered at the original configuration points. The short time Green's function is a normalized gaussian multiplied by a factor

$$W(R') = \exp(-(V(R')-E_T)\Delta\tau). \tag{23}$$

This weighting factor is the probability that the configuration will survive a time $\Delta\tau$ in the presence of an absorption probability $V(R')-E_T$. If $W<1$, then with probability 1-W, that configuration is eliminated from the simulation. Since $V(R')$ can be less than E_T, W may be greater than one. This is a branching ratio, or more precisely, the expected number of new configurations generated in a time $\Delta\tau$. Thus for $1<W<2$, a second configuration is sampled with probability W-1. For W greater than two, the generalization is obvious. After one has sampled 0, 1, or more configurations from each initial configuration, a new population of points has been obtained, and these points have been sampled from $\psi(R,\Delta\tau)$ (actually $P(R,\Delta\tau)$). This process has achieved one iteration of equation 13. The process is then repeated to obtain $\psi(R,2\Delta\tau)$ and may be iterated to arbitrarily large times.

Importance Sampling

Obtaining a population of points sampled from the ground state wave function is not enough to allow the calculation of expectation values. To state it simply, one cannot calculate the square of the wave function from the known set of configurations. Although the energy may be crudely obtained by adjusting the value of E_T so that the number of points in the population is stable, this estimate of E_0 has large statistical uncertainty. The random fluctuations in the size of the population due to the continual creation and annihilation of configurations can be largely eliminated through importance sampling. The philosophy at work here is the more information about the wave

function which you put into the calculation, the more effective the GFMC method is in obtaining the results. The information is a reasonably good approximate analytic form for the ground state wave function $\psi_T(R)$. This is typically a Jastrow type wave function which incorporates some short range pair correlations, a feature particularly important in coulomb systems, or systems interacting with unbounded potentials.

Using the trial wave function $\psi_T(R)$, one forms the new density,

$$f(R,\tau) = \psi(R,\tau)\ \psi_T(R) \tag{24}$$

and the new propagator

$$K(R,\tau,R',\tau') = \psi_T(R)\ G(R,\tau,R',\tau')/\psi_T(R')$$

which then satisfies the modified propagator equation,

$$f(R,\tau) = \int K(R,\tau,R',\tau')\ f(R',\tau')dR'. \tag{25}$$

This equation says that if a set of configurations is propagated forward in time according to the modified stochatic dynamics of the kernal K, then this new population eventually evolves to

$$\lim_{\tau\to\infty} f(R,\tau) \propto \phi_0(R)\ \psi_T(R). \tag{26}$$

Before discussing the modified propagation procedure and its effect on population stability, it is pointed out the secondary advantage of using $f(R,\tau)$ in the calculation of the energy. If we calculate the expected value of $(H\psi_T(R))/\psi_T(R) \equiv E(R)$ over M configurations the expression is

$$\langle (H\psi_T)/\psi_T \rangle = (1/M) \sum_{i=1}^{M} H\psi_T(R_i)/\psi_T(R_i). \tag{27}$$

This is an estimator for the expectation value over the probability density

$$P(R,\tau) = f(R,\tau)/\int dR f(R,\tau). \tag{28}$$

The average equals the ground state energy when $f(R) \propto \phi_0(R)\ \psi_T(R)$. The expectation value

$$\left\langle \frac{H\psi_T}{\psi_T} \right\rangle = \frac{\int dR \phi_0(R)\psi_T(R)\ [H\psi_T(R)/\psi_T(R)]}{\int dR \phi_0(R)\psi_T(R)} \tag{29}$$

$$= E_0 = \frac{\int dR \phi_0(R) H\psi_T(R)}{\int dR \phi_0(R)\psi_T(R)} \tag{30}$$

by the hermitian property of H. It can be shown [12] that the expectation value of E(R) is an upperbound to E_0 at any τ. The energy calculated in this fashion has a much lower statistical variance if an accurate ψ_T is known. Indeed, the statistical uncertainty would be zero if $\psi_T = \phi_0$.

The difference in the propagators K and G can be made clear if one expands the ratio $\psi(R_2)/\psi(R_1)$ using

$$\ln \psi(R_2) = \ln \psi(R_1) + (R_2-R_1)\cdot \frac{d}{dR_1} \ln \psi(R_1) + \frac{1}{2}(R_2-R_1)^2 \frac{d^2}{dR_1^2} \ln \psi(R_1). \quad (31)$$

Then, K is approximately given by

$$K = G(R,\tau,R',\tau') \exp[\ln\psi_T(R) - \ln\psi_T(R')] \quad (32)$$

$$= (1/2\pi\Delta\tau^*)^{3N/2}\exp\{-(R-(R'-F\Delta\tau^*))^2/2\Delta\tau^* - (E(R')-E_T)\Delta\tau^*\}$$

where $F = \vec{\nabla}'\ln\psi(R')$ and $\Delta\tau^* = \Delta\tau/(1-\nabla^2\ln\psi(R'))$.

This expression is correct to order $\Delta\tau$ as before, and we have neglected some cross terms of the order $(R-R')^2$ in the Taylor series expansion. This is consistent since $(R-R')^2 \sim \Delta\tau$. In this form, we see that if the trial function ψ_T is exactly equal to ϕ_0, then $E(R) = E_0$ and provided $E_T = E_0$, the propagator is a normalized gaussian. Hence the size of the population never changes and all configurations survive each step with probability W=1. When ψ_T is close to ϕ_0, the population fluctuates, but the fluctuations are much smaller. The dynamics of the diffusion have been changed by translating the center of the gaussian by an amount $F\Delta\tau^*$ towards regions of larger ψ_T, i.e. higher probability. The width of the gaussian has also changed. The population stability has been gained but at the expense of calculating E(R) at each step rather than V(R). The overall result is still a much more efficient, lower variance calculation.

THE BIEXCITON

The biexciton in its ground state consists of two electrons of opposite spin and two holes of opposite spin. The existence of the entity is without question, but its binding energy has been debated [16] and even accurate variational calculations [16] have given only 50% of the experimental binding energy in silicon and germanium. From the variational calculations of Brinkman, Rice, and Bell [16] we know that wave functions which incorporate some particle correlations yield improved binding energies. One might expect then that a GFMC calculation, which incorporates all correlation effects, would obtain significantly greater binding energies and resolve the discrepancies with experimental results.

To eliminate uncertainties in materials parameters it is best to establish a system of units where energy is measured in units of the exciton energy, E_x, given by

$$E_x = \mu e^4/2\hbar^2\kappa^2 \quad (33)$$

where μ is the reduced mass and K the dielectric constant. In these units, the four-particle Hamiltonian becomes

$$H = -(1/(1+\sigma))(\nabla_1^2 + \nabla_2^2) - (\sigma/(1+\sigma))(\nabla_a^2 - \nabla_b^2)$$

$$+ 2/r_{12} + 2/r_{ab} - 2/r_{1a} - 2/r_{1b} - 2/r_{2a} - 2/r_{2b} \qquad (34)$$

where, $\sigma = m_e/m_h$, and the electron coordinates are labeled 1,2 and the hole coordinates a,b.

The trial wave function, $\psi_T(R)$ was the product of three functions ψ_{ee}, ψ_{hh} and ψ_{eh}, chosen to incorporate as much information about pair correlations as possible.

$$\psi_{ee}(r) = \exp[c_1 r/(1+c_2 r)]$$

$$\psi_{hh}(r) = \exp[c_3 r/(1+c_4 r)]$$

$$\psi_{eh} = \exp[-(\alpha r_{1a} + \beta r_{1b} + \beta r_{2a} + \alpha r_{2b})]$$

$$+ \exp[-(\beta r_{1a} + \alpha r_{1b} + \alpha r_{2a} + \beta r_{2b})] \qquad (35)$$

The GFMC calculations were performed for several values of the mass ratio, $\sigma = 0.01$, 0.1, 0.3, 0.6 and 1.0. The variational parameters c_1, c_2, c_3, c_4 and α and β were varied until a reasonable initial energy was obtained at each σ. Populations of ~500 configurations were run for typically 40 units of time with time steps of $\Delta\tau = .005$ or less. Tests were done on time steps of $\Delta\tau = .01$ and .001 to establish that the error due to the short time approximation was less than the statistical uncertainty (<0.1%) of the total energy.

Figure 1 shows the results from the GFMC calculations and the results of the variational calculations of ref. 16. In these units, the energy of two isolated excitons is -2.0. One sees that as the electron and hole masses become comparable the system becomes weakly bound. When $\sigma = 1$, the binding energy is about 3% of the total energy. It is in this equal mass limit that the variational calculations suffer most from inadequate treatment of correlations in the wave function, and yield a binding energy of only half the correct value. The 1-2% error in the total variational energy becomes less important as the hole mass increases.

Comparison of the GFMC results to experimental measurements can be made for several values of σ. For small σ an exact form for the energy is known [17],

$$E(\sigma) = (-2.346 + 0.764\sqrt{\sigma})E_x \qquad (36)$$

and agrees with the GFMC results at $\sigma = .01$ to better than three significant figures. In this mass range CuBr and CuCl [2,18] have values of $\sigma = 0.01$ and 0.02 and experimental binding energies of ~29 mev and 34-44 mev respectively.

The exciton energies of 110 and 190 mev in these systems give GFMC energies of 29 and 45 mev respectively. This is very good agreement, but it must be treated cautiously since a small uncertainty in the mass makes a big change in the energy in this region of small σ. A more reasonable comparison may be to take the measured binding energy and predict the mass ratio, since it is the less accurate quantity.

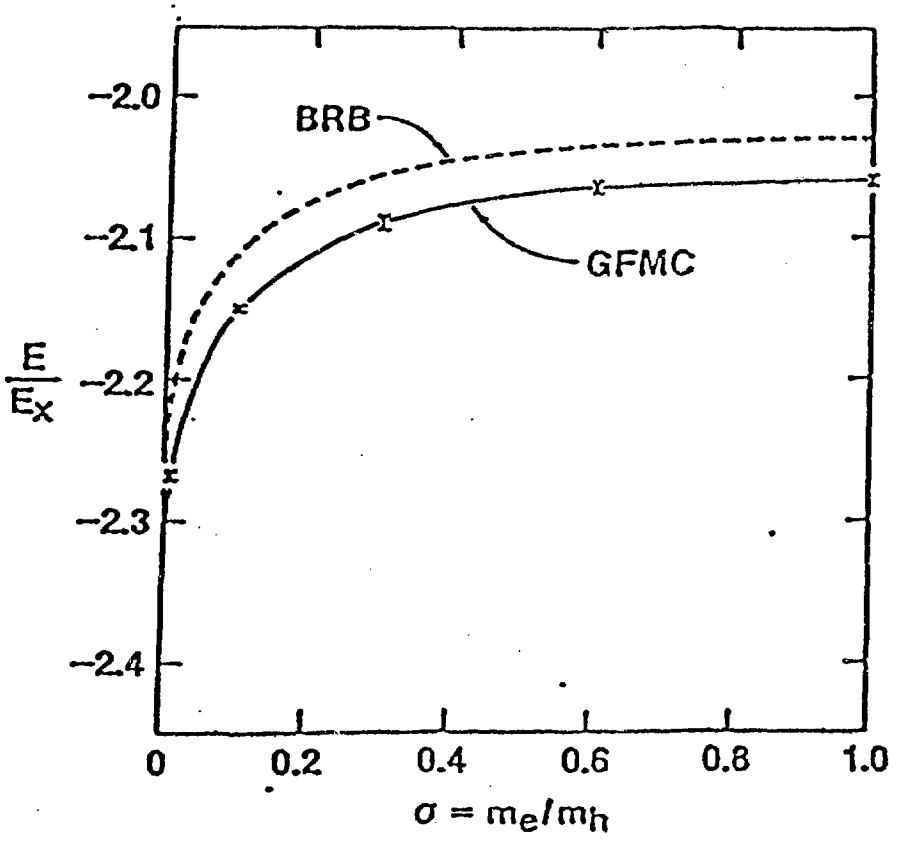

Figure 1. Ground-state energy of biexcitons as a function of the electron-hole ratio, σ. The dotted curve represents the variational results of Brinkman, Rice and Bell (BRB) (ref. 16) while the solid curve shows the Green's Function Monte Carlo (GFMC) results. Here the energies are expressed in excitonic rydbergs, E_x.

Germanium and silicon are well studied systems and have electron-hole masses which are more nearly equal. There is, however, the complication of band warping since the top of the two valence bands in these semiconductors are degenerate and coupled. Recently biexcitons have been observed stressed Ge<1,1,16> [19] and Si<1,0,0> [3] where the electrons occupy a single conduction band and the holes occupy a single hole band. These bands are anisotropic, but we will come back to that point later. In the germanium experiments the binding energy is estimated to be .15 ± .01 mev and using σ = .7, the GFMC

energy corresponds to a .16 mev binding energy. The variational calculation obtains only 60% of this binding. In the experiments on stressed Si<100>, Gourley and Wolfe [3] report the binding energy to be 0.10 E_x which is to be compared with a value of 0.08 E_x in unstressed Si [20] and a GFMC value of .06 E_x when a mass ratio of $\sigma \sim 1$ is taken.

It is only in silicon that there appears to be a discrepancy between calculated and experimental results. The variational result accounts for about 1/3 of the binding and the GFMC accounts for about 2/3 of the observed binding energy. This is one of the advantages of an exact numerical result. A discrepancy with experiment tells you something, because it cannot be attributed to approximations invoked in arriving at the solution of the problem. In the present case we have essentially an exact result for the ground state energy of the effective mass Hamiltonian. Apparently, this Hamiltonian does not exactly correspond to the experimental system. One difference is that the calculation has not included band anisotropy. Because the curvature of both the electron and hole bands is different along different crystal axes, the effective masses along these axes must be distinguished as to the longitudinal m_l and transverse m_T components. Returning for a moment to the analogy between the Schroedinger equation and a diffusion equation, this is equivalent mathematically to saying that the system has an anisotropic diffusion constant. This feature makes even the two-body exciton Hamiltonian insolvable analytically but causes only a minor change in the GFMC calculation. We have accordingly taken literature values [21] of the anisotropic masses in silicon, and repeated the silicon calculations to determine the effect of this anisotropy. Preliminary results indicate that at most the binding energy is lowered another 10% removing perhaps a third of the remaining discrepancy. Compared to the total energy this is a small difference ~1.5%. One may even take this result as support for the surprising accuracy of the effective mass Hamiltonian. Alternatively one may use it to motivate an attempt to find the physical origins of the additional binding energy.

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