Quantization of exciton in magnetic field background

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(Dated: February 2, 2008)

The possible mismatch between the theoretical and experimental absorption of the edge peaks in semiconductors in a magnetic field background may arise due to the approximation scheme used to analytically calculate the absorption coefficient. As a possible remedy we suggest to consider nontrivial boundary conditions on $x$-$y$ plane by inequivalently quantizing the exciton in background magnetic field. This inequivalent quantization is based on von Neumann’s method of self-adjoint extension, which is characterized by a parameter $\Sigma$. We obtain bound state solution and scattering state solution, which in general depend upon the self-adjoint extension parameter $\Sigma$. The parameter $\Sigma$ can be used to fine tune the optical absorption coefficient $K(\Sigma)$ to match with the experiment.

PACS numbers: 03.65.Ge, 71.35.-y, 71.35.Cc, 03.65.Db

I. INTRODUCTION

Exciton\textsuperscript{1} is a bound pair between an electron and a hole in a crystal, which interact through Coulomb attraction between them. When an electron from the valence band is excited into the conduction band, the missing electron in the valence band leaves a hole with opposite electric charge. The exciton results from the binding of the electron with its hole. As a result the exciton has slightly less energy than the unbound electron and hole. It has an important role to play in the fine structure of the absorption edge in semiconductor. It has been seen that as the photon energy goes above the band gap energy of the semiconductor, the absorption coefficient shows spikes due to the formation of exciton\textsuperscript{2}. This is an important study no doubt, because it explores the band structure and the character of the one electron states of the semiconductor. The properties of a semiconductor are mostly determined by the electronic states which lie just below and just above the forbidden gap.

An appreciable amount of studies have been made to explore the band structure of semiconductors by examining direct and indirect optical absorption in semiconductors\textsuperscript{3}. This absorption may arise due to the transition between the states of the same side of the forbidden gap or across the forbidden gap.

There have been a lot of studies in this field both theoretically and experimentally, see for example\textsuperscript{4,5}. Since the constituents of exciton are electrically charged, the magnetic fields have certain effects on the energy spectra of the exciton and it in turn affects the fine structure of the absorption. The magnetic fields have a Zeeman like effect on the energy spectra of an exciton, which has been investigated by studying optical absorption in many substances, for example, in InSb\textsuperscript{6}, Ge and InAs. Magneto-optic effect in strained and unstrained Ge\textsuperscript{7} have been performed in\textsuperscript{7}. In\textsuperscript{8}, a theoretical study of the effect of magnetic field on the absorption edge in solid has been done, neglecting the Coulomb interaction between the electron and the hole. It is shown that a series of peaks may form due to the transition between the sub-bands, which originate due to the splitting of electron energy states in the solid by the magnetic field. Instead of forming peaks, in some cases a series of steps are formed due to magnetic field. But Coulomb interaction certainly has effect\textsuperscript{9} on the absorption in solids. It is therefore required to consider Coulomb interaction and magnetic field simultaneously in the study of absorption\textsuperscript{10}. In general this problem is hard to tackle analytically for any magnetic field. But for large magnetic field an approximation scheme\textsuperscript{10} can be used to handle the situation and can be checked experimentally for some substances like InSb, Ge etc. According to this approximation scheme, which is valid in large magnetic field, the Coulomb term should only affect the dynamics of the exciton in the direction of the applied magnetic field and it is therefore possible to reduce the time independent three dimensional Schrödinger equation into one dimensional eigenvalue equation in the direction of the magnetic field. The inclusion of the Coulomb interaction shows that the the absorption peaks in each magnetic sub-band transition is moved towards the lowest exciton line. The other effects are the reduction of intensity of the continuous absorption and to smooth out the peaks near the absorption edge. The peaks are the exciton peaks instead of the magneto-optic peaks.

It is expected that the analytical theory of absorption in solids\textsuperscript{10} will not be able to exactly explore the true nature of the band structure due to the approximation used in the calculation. In this article, we therefore try to incorporate some short range interactions into the boundary condition, imposed on the domain of the system so that the results based on the approximate model agrees with the experiments as much as possible. This nontrivial boundary condition will in general change the energy spectrum of the system and it will depend on a parameter, called self-adjoint extension parameter. The fine structure of the optical absorption edge in a crystal due to exciton essentially depends on the energy spectrum.

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of the exciton. It is therefore expected to change if the spectrum changes. To get a consistent boundary condition and the domain, so that the Hamiltonian remains self-adjoint, we perform a self-adjoint extension (SAE) of the one dimensional Hamiltonian in the direction of the magnetic field by using von Neumann’s method \[11\]. Self-adjointness of a Hamiltonian is essential, because otherwise the Hamiltonian would generate complex eigenvalues and the time evolution of the states will not be unitary. SAE has received lot of interests in recent years and is now being used extensively in different branches of physics, to explore the nontrivial quantum behavior of different systems \[12, 13, 14, 15, 16, 17, 18\].

The present article has been organized as follows: In sec. II, we discuss about the exciton in a magnetic field background and write an effective radial eigenvalue equation following \[10\], which we need to quantize using nontrivial boundary condition. The method of self-adjoint extensions (SAE) is discussed in Sec. III, which is essential to get nontrivial boundary condition for the effective Hamiltonian \(H_{|z|}\) so that the Hamiltonian is self-adjoint. The bound state and scattering state solutions are discussed in Sec. IV and V respectively. We conclude the paper with a discussion in Sec VI.

II. EXCITON IN MAGNETIC FIELD BACKGROUND

We consider dynamics of electron and hole pair with effective masses \(m_e\) and \(m_h\) respectively in a medium of dielectric constant \(\kappa\). In a magnetic field background \(\mathbf{B}\) the time independent Schrödinger equation for the system is given by \[10\]

\[
\left[ \frac{1}{2m_e} \left( \mathbf{p} + \frac{e}{c} \mathbf{A}(\mathbf{r}_e) \right)^2 + \frac{1}{2m_h} \left( \mathbf{p} - \frac{e}{c} \mathbf{A}(\mathbf{r}_h) \right)^2 - \frac{e^2}{\kappa|\mathbf{r}_e - \mathbf{r}_h|} \right] \Psi = E \Psi ,
\]

where \(\mathbf{A}(\mathbf{r}_e)\) and \(\mathbf{A}(\mathbf{r}_h)\) are magnetic vector potentials at electron and hole positions respectively.

Considering the fact that the states of interest in optical transitions are only those in which \(\mathbf{k} = \mathbf{k}_e + \mathbf{k}_h = 0\) (where \(\mathbf{k}_e\) and \(\mathbf{k}_h\) are electron and hole wave vectors respectively) by changing the variables to the center of mass coordinate \(\mathbf{p} = m_e \mathbf{p}_e + m_h \mathbf{p}_h/m_e + m_h\) and relative position \(\mathbf{r} = \mathbf{r}_e - \mathbf{r}_h\) and using the substitution \(\Psi(\mathbf{r}_e, \mathbf{r}_h) = U(\mathbf{r}) \exp\left[-\frac{ie}{2\kappa c} \mathbf{B} \times \mathbf{p} \cdot \mathbf{r} \right]\)

\[
\begin{align*}
\frac{\hbar^2}{2\mu} \nabla^2 - \frac{ie\hbar}{2c} \left( \frac{1}{m_e} - \frac{1}{m_h} \right) \mathbf{B} \cdot \nabla + \frac{e^2}{8\mu c^2} (\mathbf{B} \times \nabla)^2 - \frac{e^2}{\kappa r} U(\mathbf{r}) = EU(\mathbf{r}),
\end{align*}
\]

where \(\mu\) is the reduced mass \(\mu = m_e m_h/(m_e + m_h)\) of the electron-hole system. The presence of Coulomb interaction spoils the separability of \[2\] in any co-ordinates. So it is difficult to solve the equation in any coordinate system. It can however be reduced in an one dimensional eigenvalue equation in large magnetic field limit. Note that the magnetic field affects the motion of a charged particle in a direction perpendicular to the magnetic field. In our case we take the magnetic field in \(z\) direction. So, in \(z\) direction the charged particle motion will be a free particle motion in absence of Coulomb force. But in presence of Coulomb force the free motion in \(z\) direction will be modified according to Ref. \[20\]. The potential along \(z\) direction will now be the average Coulomb potential over the \(x\)-\(y\) plane at each point in \(z\) axis \[10\]. From now on, we take \(\hbar^2 = 2\mu = e^2 = 1\), for the simplicity of calculations. In these units, the one dimensional Differential Equation is of the form \[10\]

\[
H_{|z|}(\chi(|z|)) = -\frac{d^2\chi}{|z|^2} - \left[ \frac{1}{\kappa(a + |z|)} - \frac{Aa}{\kappa(a + |z|)^2} \right] \chi(|z|)
= E_{|z|}\chi(|z|),
\]

where \(a\) and \(A\) are constant parameters (see Ref. \[10\] for details) and its values will depend on the eigenfunctions on the perpendicular \(x\)-\(y\) plane. We thus lead to a one dimensional differential eigenvalue problem which depends on the modulus of Cartesian co-ordinate \(z\) due to the reflection symmetry on the \(z\) axis. The inner product is now defined as

\[
(\chi_1(|z|), \chi_2(|z|)) = \int_0^{\infty} \chi_1(|z|)\chi_2(|z|)|z|dz
\]

(4)

where \(|z|\) is the measure. In order to find the bound state eigenvalue and corresponding eigenfunction of \[3\], we need to consider a physically meaningful boundary condition. We want to find out this boundary condition by von Neumann’s method of self-adjoint extension (SAE).

III. VON NEUMANN’S METHOD OF SAE

Before going into the actual Hamiltonian \(H_{|z|}\) of \[3\], it is essential to discuss about the general properties and method of self-adjoint extensions of an operator \(\mathcal{B}\) defined over the elements of a Hilbert space \(\mathcal{H}\). Let us consider \(\mathcal{D}(\mathcal{B})\) as the domain of \(\mathcal{B}\) such that the operator \(\mathcal{B}\) becomes symmetric in that domain. The operator \(\mathcal{B}\) is said to be symmetric (or hermitian) if it satisfies the condition \((\mathcal{B}\phi_1, \phi_2) = (\phi_1, \mathcal{B}\phi_2), \forall \phi_1, \phi_2 \in \mathcal{D}(\mathcal{B})\), where \((\ldots)\) is the inner product defined over the Hilbert space. Given the operator \(\mathcal{B}\) and the inner product \((\ldots)\), one can calculate the adjoint operator \(\mathcal{B}^*\) from the Green’s formula \[21\]. This adjoint operator \(\mathcal{B}^*\) should have a domain \(\mathcal{D}(\mathcal{B}^*)\), which can be obtained from \((\mathcal{B}^*\phi_1, \phi_2) = (\phi_1, \mathcal{B}\phi_2), \forall \phi_1, \phi_2 \in \mathcal{D}(\mathcal{B}), \mathcal{B}\phi_1 \in \mathcal{D}(\mathcal{B})\). Now, if the operator is self-adjoint then \(\mathcal{D}(\mathcal{B}) = \mathcal{D}(\mathcal{B}^*)\) and for non self-adjoint case \(\mathcal{D}(\mathcal{B}) \neq \mathcal{D}(\mathcal{B}^*)\). For non self-adjoint operators we
need to find out self-adjoint extensions, because according to Stone’s theorem self-adjointness of an operator is necessary in order to guarantee unitary evolution. We follow von Neumann’s method for finding self-adjoint extensions of the Hamiltonian, if there is any. According to this method, we first need to find out the solutions of the equation \( \mathcal{B}^* \phi^\pm = \pm i \phi^\pm \). \( \phi^\pm \) are called deficiency space solutions, because the numbers \( n^\pm \) are a measure by which a non self-adjoint operator is away from self-adjointness, where \( n^\pm \) denotes the number of \( \phi^\pm \) solutions. For \( n^+ = n^- = 0 \), the operator \( \mathcal{B}^* \) is self-adjoint. For \( n^+ = n^- = n \neq 0 \), the operator \( \mathcal{B}^* \) is not self-adjoint, but admits self-adjoint extensions characterized by \( n^2 \) parameters of \( U(n) \). Finally, for \( n^+ \neq n^- \), the operator \( \mathcal{B}^* \) is not self-adjoint and can’t be made self-adjoint. The self-adjoint extension of the operator \( \mathcal{B}^* \) is given by the domain \( \mathcal{D}_{U(n)}(B) \equiv \phi + \phi^+ + U(n)\phi^- \), where \( \phi \in \mathcal{D}(B) \).

### IV. Bound State Solution of Exciton

We now come to the discussion of the Hamiltonian \( \Sigma \), for which we seek a self-adjoint domain. We construct an initial domain \( \phi(|z|) \in \mathcal{D}(H_{|z|}) \), where \( \phi(|z|) \) and \( \phi'(|z|) \) are absolutely continuous and \( \phi(0) = \phi'(0) = 0 \). It is implied that \( \phi(|z|) \) and \( H_{|z|}\phi(|z|) \) are square-integrable functions, i.e., belong to the Hilbert space. Note that \( \mathcal{D}(H_{|z|}) \) is so restricted that the Hamiltonian \( H_{|z|} \) becomes symmetric in this domain. The adjoint Hamiltonian \( H_{|z|}^* \) has the same differential form \( [3] \), but the domain is given by \( \phi(|z|) \in \mathcal{D}(H_{|z|}^*), \) where \( \phi(|z|) \) and \( \phi'(|z|) \) are absolutely continuous. The two domains are seen to be different, i.e., \( \mathcal{D}(H_{|z|}) \neq \mathcal{D}(H_{|z|}^*). \) So we need to find out the deficiency space solutions (square integrable), which are in our case the solutions of the differential equations \( H_{|z|}^* \phi^\pm = \pm i \phi^\pm \). These are

\[
\phi^\pm(|z|) = W_{\alpha^\pm,m} \left( \frac{1}{\kappa \alpha^\pm} (a + |z|) \right),
\]

where \( \alpha^\pm = \pm \frac{i}{\kappa} e^{\mp i \pi/4} \) and \( m = \sqrt{\left( \frac{a}{\kappa} \mp \frac{B}{\kappa} \right)} \) and \( W \) is the Whittaker’s function \([22]\). The square integrability of \( \phi \) can be easily checked from the asymptotic and short distance behavior. Note however that the potential at \( |z| \to 0 \) is always finite so there is no problem of short distance square-integrability but the short distance behavior will help to get the spectrum for the problem. The asymptotic behavior is given by

\[
\lim_{|z| \to \infty} \phi^\pm(|z|) \simeq \left( \frac{1}{\kappa \alpha^\pm} (a + |z|) \right)^{\alpha^\pm} \exp\left( -\frac{1}{2 \kappa \alpha^\pm} (a + |z|) \right),
\]

which goes to zero asymptotically, i.e., \( \phi^\pm(|z|) \to 0 \). In order to get short distance behavior we need to express the Whittaker’s function in terms of Kummer function as

\[
W_{a,b}(z) = e^{-\frac{1}{2} z} z^{\frac{a + b}{2} - \frac{1}{2}} \frac{\pi}{\sin \pi a} \left[ \frac{M(\frac{1}{2} + b - a, 1 + 2b, x)}{\Gamma(\frac{1}{2} - a - b)\Gamma(1 + 2b)} - z^{2b} \frac{M(\frac{1}{2} - a - b, 1 - 2b, x)}{\Gamma(\frac{1}{2} + b - a)\Gamma(1 - 2b)} \right],
\]

where \( M \) is the Kummer function \([22]\). The short distance behavior can now be evaluated as

\[
\lim_{|z| \to 0} \phi^\pm(|z|) \simeq \left[ A^\pm (a + |z|)^{1/2 + m} - B^\pm (a + |z|)^{1/2 - m} \right],
\]

where \( A^\pm = \frac{\pi}{\sin \pi (1 + 2m)(1/2 - \alpha^\pm - m)\Gamma(1 + 2m)} \) and \( B^\pm = \frac{\pi}{\sin \pi (1 + 2m)(1/2 - \alpha^\pm + m)\Gamma(1 - 2m)} \).

Since in our case \( n^+ = n^- = 1 \), \( H_{|z|} \) is not self-adjoint but it admits self-adjoint extensions, characterized by a parameter \( \Sigma \) and the domain over which the Hamiltonian \( H_{|z|}^\Sigma \) is self-adjoint is given by

\[
\mathcal{D}(H_{|z|}^\Sigma) = \{ \phi(|z|) + \phi^+(|z|) + \exp(i \Sigma) \phi^-(|z|) \},
\]

where \( \phi(|z|) \in \mathcal{D}(H_{|z|}) \). Now we can solve the eigenvalue problem \([19]\) and find out eigenvalue using the extended domain \([19]\). The eigenfunction of \([19]\) apart from normalization is given by

\[
\chi(|z|) = W_{\alpha,m} \left( \frac{1}{\kappa \alpha} (a + |z|) \right),
\]

where \( \alpha = \frac{1}{\kappa} \sqrt{\frac{1}{2} - \frac{B}{\kappa}} \) and \( m \) has already been defined. The eigenvalue of \([19]\) can be found by looking at the short distance behavior of \([19]\) and \([19]\) and equating the coefficients of equal powers of \( (a + |z|) \). For general value of the self-adjoint extension parameter \( \Sigma \), the eigenvalue equation is found to be

\[
f(E_{|z|}) = \frac{\Gamma(1/2 + m - \alpha)}{\Gamma(1/2 - m - \alpha)} = \frac{\chi_1 \cos(\theta_1 - \Sigma/2)}{\chi_2 \cos(\theta_2 - \Sigma/2)},
\]

where \( \Gamma(1/2 - m - \alpha^+) = \chi_1 \exp(-i \theta_1) \) and \( \Gamma(1/2 + m - \alpha^+) = \chi_2 \exp(-i \theta_2) \). The eigenvalue equation \([19]\) is a
1-parameter family of equation. It is to be noted that the equation of the form (11) is discussed in detail in Ref. [13, 23] and the reason we get similar equation here is that the nature of the boundary condition obtained from the short distance behavior of the special functions are similar in both cases. Each value of the parameter $\Sigma$ correspond to a different quantization for the system. A plot of $f(E_{\pm})$ as a function of $\Delta$ can be evaluated exactly. For example, when the R.H.S of (14) from Eq. (13), but this time $\Sigma = 1$.

We now move to the discussion of scattering state solutions. The eigenvalue equation for scattering states will be the same Eq. (3), where $E_{\pm}$ is now positive. The scattering state solution is of the form

\[ \chi(|z|) = C(i\tilde{\alpha})M_{i\tilde{\alpha},m} \left( \frac{1}{i\kappa\alpha}(a + |z|) \right) + D(i\tilde{\alpha})W_{i\tilde{\alpha},m} \left( \frac{1}{i\kappa\alpha}(a + |z|) \right) \]  

where $\tilde{\alpha} = \frac{1}{2\pi} \sqrt{\frac{1}{E_{\pm}}}$ and $C(i\tilde{\alpha})$ and $D(i\tilde{\alpha})$ are undetermined coefficients. One can now determine the coefficients $C$ and $D$ by looking at the short distance behavior of (9) and (15) and equating the same powers of $(a + |z|)$, which will now depend upon the self-adjoint extension parameter $\Sigma$. Note that the scattering state solution (15) does not belong to the domain $|\tilde{\alpha}|$ for the simple reason that the scattering state solutions are not normalizable and thus does not belong to the Hilbert space. But there is no problem for the scattering states to be square integrable at short distance and thus it may belong to the domain $|\tilde{\alpha}|$ as far as the short distance behavior is concerned (see [11] for detail discussion with an example) It is also possible to calculate the $S$-matrix and phase shift from this scattering state solution.

VI. DISCUSSION

The knowledge of quantum mechanical behavior of exciton in a magnetic field background is essential for the study of absorption in semiconductors as has been shown in Ref. [10]. Since the time independent Schrödinger equation for the exciton cannot be exactly solved, an approximation scheme is generally used [10] in order to solve the system analytically. In order to overcome the shortcomings of the approximation scheme and to guarantee unitary evolution of the system we obtain a 1-parameter family of self-adjoint extensions of the effective one dimensional eigenvalue equation. We obtain bound state and scattering state solutions, which in general depend on the self-adjoint extension parameter $\Sigma$. The direct optical absorption coefficients $K(\Sigma)$ depend upon the bound and scattering state solutions which are dependent on the boundary conditions characterized by the parameter $\Sigma$. Therefore the parameter $\Sigma$ can be used to fine tune the optical absorption coefficient $K(\Sigma)$ to match with the experimental data. Our procedure gives all possible solutions for the system.

[1] J. Frenkel, Phys. Rev. 37, 17 (1931).
[2] R. J. Elliott, Phys. Rev. 108, 1384 (1957).
[3] L. H. Hall, J. Bardeen and F. J. Blatt, Phys. Rev. 95, 559 (1954); G. G. Macfarlane and V. Roberts, Phys. Rev. 97, 1714 (1955); G. G. Macfarlane and V. Roberts, Phys. Rev. 98, 1865 (1955);
[4] E. J. Johnson, Phys. Rev. Lett. 19, 352 (1967); A. Baldereschi and N. O. Lipari, Physical Review Letters 25 373 (1970); M. Altarelli and N. O. Lipari, Phys. Rev. B7, 3798 (1973); M. Altarelli and N. O. Lipari, Phys. Rev. B9, 1733 (1974); W. C. Dash and R. Newman, Phys. Rev. 99, 1151 (1955); H Y Fan, Rep. Prog. Phys. 19, 107 (1956).
W. Andreoni, M. Altarelli, and F. Bassani, Phys. Rev. B 11, 2352 (1975).
[5] J. Maultzsch et. al, Phys. Rev. B 72, 241402(R) (2005); S. Zaric et. al, Phys. Rev. Lett. 96, 016406 (2006); S. Uryu and T. Ando, Phys. Rev. B 74, 155411 (2006); S. Uryu and T. Ando, Phys. Rev. B 76, 115420 (2007).
[6] E. Burstein and G. S. Picus, Phys. Rev. 105, 1123 (1957).
[7] D. F. Edwards and V. J. Lazazzera, Phys. Rev. 120, 420 (1960).
[8] R. J. Elliott, T.P. Mclean and G.G. Macfarlane, Proc. Phys. Soc. Lond. 72, 553 (1958).
[9] G. Dresselhaus, Phys. Rev. 106, 76 (1957); R. J. Elliott, Phys. Rev. 108, 1384 (1957).
[10] R. J. Elliott and R. Loudon, J. Phys. Chem. Solids.8, 382 (1959); R. J. Elliott and R. Loudon, J. Phys. Chem. Solids.15, 196 (1960).
[11] M. Reed and B. Simon, Fourier Analysis, Self-Adjointness II ( New York:Academic, 1975 ).
[12] B. Basu-Mallick, Pijush K. Ghosh and Kumar S. Gupta, Nucl. Phys. B659, 437 (2003).
[13] B. Basu-Mallick, Pijush K. Ghosh and Kumar S. Gupta, Phys. Lett. A311, 87 (2003).
[14] Kumar S. Gupta, Mod. Phys. Lett. A18, 2355 (2003).
[15] B. Basu-Mallick and Kumar S. Gupta, Phys. Lett. A292, 36 (2001).
[16] S. Meljanac, A. Samsarov, B. Basu-Mallick and Kumar S. Gupta, Eur. Phys. J. C49, 875 (2007).
[17] P. R. Giri, K. S. Gupta, S. Meljanac and A. Samsarov, hep-th/0703121.
[18] D. Birmingham, Kumar S. Gupta and Siddhartha Sen, Phys. Lett. B505, 191 (2001); Kumar S. Gupta and Siddhartha Sen, Phys. Lett. B526, 121 (2002).
[19] W. Lamb, Phys. Rev. 85, 259 (1952).
[20] L. I. Schiff and H. Snyder, Phys. Rev. 55, 59 (1939).
[21] N. Dunford and J. T. Schwartz, Linear Operators, Spectral Theory, Self-Adjoint Operators in Hilbert Space, Part 2 (Wiley-Interscience, 1988).
[22] M. Abromowitz, I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1970).
[23] L. Feher, I. Tsutsui and T. Fulop, Nucl. Phys. B715, 713 (2005).