Chapter 4
Solution Manual

Written by: Albert Liu

4.1:

The time-independent Schrodinger equation for the hydrogen atom is given by:

$$\left[-\frac{\hbar^2}{2m_p}\nabla_p^2 - \frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{e^2}{4\pi\epsilon|\mathbf{r}_p - \mathbf{r}_e|}\right]\psi(\mathbf{r}_p, \mathbf{r}_e) = E\psi(\mathbf{r}_p, \mathbf{r}_e) \tag{1}$$

The center of mass and relative coordinates $\mathbf{r}_{cm}$ and $\mathbf{r}_{rel}$ respectively are given by:

$$\mathbf{r}_{cm} = \frac{m_p\mathbf{r}_p + m_e\mathbf{r}_e}{m_p + m_e} \qquad \mathbf{r}_{rel} = \mathbf{r}_p - \mathbf{r}_e \tag{2}$$

We can express $\mathbf{r}_p$ and $\mathbf{r}_e$ in terms of $\mathbf{r}_{cm}$ and $\mathbf{r}_{rel}$:

$$\mathbf{r}_p = \mathbf{r}_{cm} + \frac{m_e}{m_p + m_e}\mathbf{r}_{rel} \qquad \mathbf{r}_e = \mathbf{r}_{cm} - \frac{m_p}{m_p + m_e}\mathbf{r}_{rel} \tag{3}$$

Noting that the second derivatives can be transformed as:

$$\begin{aligned}
\frac{d^2}{dx_p^2} &= \frac{d}{dx_p}\left(\frac{dx_{cm}}{dx_p}\frac{d}{dx_{cm}} + \frac{dx_{rel}}{dx_p}\frac{d}{dx_{rel}}\right) \\
&= \frac{d^2x_{cm}}{dx_p^2}\frac{d}{dx_{cm}} + \left(\frac{dx_{cm}}{dx_p}\right)^2\frac{d^2}{dx_{cm}^2} + \frac{d^2x_{rel}}{dx_p^2}\frac{d}{dx_{rel}} + \left(\frac{dx_{rel}}{dx_p}\right)^2\frac{d}{dx_{rel}} \\
&= \left(\frac{m_p}{m_p + m_e}\right)^2\frac{d^2}{dx_{cm}^2} + \frac{d^2}{dx_{rel}^2} && (4) \\
\frac{d^2}{dx_e^2} &= \frac{d}{dx_e}\left(\frac{dx_{cm}}{dx_e}\frac{d}{dx_{cm}} + \frac{dx_{rel}}{dx_e}\frac{d}{dx_{rel}}\right) \\
&= \frac{d^2x_{cm}}{dx_e^2}\frac{d}{dx_{cm}} + \left(\frac{dx_{cm}}{dx_e}\right)^2\frac{d^2}{dx_{cm}^2} + \frac{d^2x_{rel}}{dx_e^2}\frac{d}{dx_{rel}} + \left(\frac{dx_{rel}}{dx_e}\right)^2\frac{d^2}{dx_{rel}^2} \\
&= \left(\frac{m_e}{m_p + m_e}\right)^2\frac{d^2}{dx_{cm}^2} + \frac{d^2}{dx_{rel}^2} && (5) \\
&\ \vdots
\end{aligned}$$

The Laplacians for the electron and proton respectively can be recast as:

$$\nabla_p^2 = \left(\frac{m_p}{m_p + m_e}\right)^2\nabla_{cm}^2 + \nabla_{rel}^2 \qquad \nabla_e^2 = \left(\frac{m_e}{m_p + m_e}\right)^2\nabla_{cm}^2 + \nabla_{rel}^2 \tag{6}$$

The Schrodinger equation can thus be rewritten in the center of mass and relative coordinates as:

$$\left[\underbrace{-\frac{\hbar^2}{M}\nabla_{cm}^2}_{\hat{H}_{cm}}\underbrace{- \frac{\hbar^2}{2\mu}\nabla_{rel}^2 - \frac{e^2}{4\pi\epsilon r_{rel}}}_{\hat{H}_{rel}}\right]\psi(\mathbf{r}_{cm}, \mathbf{r}_{rel}) = E\psi(\mathbf{r}_{cm}, \mathbf{r}_{rel}) \tag{7}$$

where we've defined the total mass M and the reduced mass μ by:

$$M = m_p + m_e \qquad \frac{1}{\mu} = \frac{1}{m_p} + \frac{1}{m_e} \tag{8}$$

4.2:

(a) We have the relative motion Hamiltonian:

$$\hat{H}_{rel} = -\frac{\hbar^2}{2\mu}\nabla^2_{rel} - \frac{e^2}{4\pi\epsilon r_{rel}} \tag{9}$$

(b) We now try a solution of the form:

$$\psi_{rel}(r_{rel}, \theta, \phi) = Ce^{-\frac{r_{rel}}{a_0}} \tag{10}$$

which gives:

$$\begin{aligned} ECe^{-\frac{r_{rel}}{a_0}} &= -\frac{\hbar^2}{2\mu}\frac{1}{r_{rel}^2}\frac{d}{dr_{rel}}\left(r_{rel}^2\frac{d}{dr_{rel}}Ce^{-\frac{r_{rel}}{a_0}}\right) - \frac{e^2}{4\pi\epsilon r_{rel}}Ce^{-\frac{r_{rel}}{a_0}} \\ &= \frac{\hbar^2}{2\mu a_0}\frac{1}{r_{rel}^2}\left(2r_{rel} - \frac{r_{rel}^2}{a_0}\right)Ce^{-\frac{r_{rel}}{a_0}} - \frac{e^2}{4\pi\epsilon r_{rel}}Ce^{-\frac{r_{rel}}{a_0}} \\ &= \frac{1}{r_{rel}}\left(\frac{\hbar^2}{\mu a_0} - \frac{e^2}{4\pi\epsilon}\right)Ce^{-\frac{r_{rel}}{a_0}} - \frac{\hbar^2}{2\mu a_0^2}Ce^{-\frac{r_{rel}}{a_0}} \end{aligned} \tag{11}$$

For our ansatz to be a solution of the Schrodinger equation, the first term on the right must vanish due to its dependence on r_{rel}, which gives the exciton Bohr radius:

$$a_0 = \frac{4\pi\epsilon\hbar^2}{\mu e^2} \tag{12}$$

Noting that the first term on the right vanishes, the eigenenergy is thus given by:

$$E = -\frac{\hbar^2}{2\mu a_0^2} = -\frac{\mu e^4}{32\pi^2\epsilon^2\hbar^2} \tag{13}$$

The normalization constant C is then given by:

$$\begin{aligned} 1 &= C^2\int_0^{\pi}\int_0^{2\pi}\int_0^{\infty} e^{-\frac{2r_{rel}}{a_0}} r_{rel}^2 sin(\theta) dr_{rel} d\phi d\theta \\ &= C^2(4\pi)\frac{a_0^3}{4} \\ \rightarrow C &= \frac{1}{\sqrt{\pi}a_0^{\frac{3}{2}}} \end{aligned} \tag{14}$$

4.3:

We have the wavefunction:

$$\psi_{rel}(r_{rel},\theta,\phi) = \frac{1}{\sqrt{\pi}a_0^{\frac{3}{2}}} e^{-\frac{r_{rel}}{a_0}} \tag{15}$$

with the probability density:

$$|\psi_{rel}|^2 = \frac{1}{\pi a_0^3} e^{-\frac{2r_{rel}}{a_0}} \tag{16}$$

The probability of finding the particle at a radius r is equivalent to the probability of finding it between a radii r and $r + dr$:

$$P = \frac{1}{\pi a_0^3} e^{-\frac{2r}{a_0}} 4\pi r^2 dr \tag{17}$$

We find the maximum probability by:

$$\begin{aligned} 0 &= \frac{dP}{dr} \\ &= \frac{4\pi dr}{\pi a_0^3}\left(2r_{max} - \frac{2r_{max}^2}{a_0}\right) e^{-\frac{2r_{max}}{a_0}} \\ \rightarrow r_{max} &= a_0 \end{aligned} \tag{18}$$

We now find the expectation value:

$$\begin{aligned} \langle r \rangle &= \frac{1}{\pi a_0^3} \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} e^{-\frac{2r_{rel}}{a_0}} r_{rel}^3 sin(\theta) dr_{rel} d\theta d\phi \\ &= \frac{3}{2} a_0 \end{aligned} \tag{19}$$

4.4:

(a) This is of the same form as the solution used in (4.2) and (4.3), which were shown to be a solution of the relative motion exciton Hamiltonian.

(b) We first find $\hat{H}_{rel}\psi_{rel}(r_{rel},\theta,\phi)$:

$$\begin{aligned} \hat{H}_{rel}\psi_{rel}(r_{rel},\theta,\phi) &= \left[-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\epsilon r_{rel}}\right] \frac{1}{\sqrt{\pi}\xi^{\frac{3}{2}}} e^{-\frac{r}{\xi}} \\ &= \frac{1}{\sqrt{\pi}\xi^{\frac{3}{2}} r_{rel}} \left(\frac{\hbar^2}{\mu\xi} - \frac{e^2}{4\pi\epsilon}\right) e^{-\frac{r_{rel}}{\xi}} - \frac{\hbar^2}{2\mu\xi^2} \frac{1}{\sqrt{\pi}\xi^{\frac{3}{2}}} e^{-\frac{r_{rel}}{\xi}} \end{aligned} \tag{20}$$

The expectation value of the energy is given by:

$$\begin{aligned} \langle E \rangle &= \iiint \psi_{rel}^* \hat{H} \psi_{rel} r_{rel}^2 sin(\theta) dr d\theta d\phi \\ &= \frac{1}{\pi\xi^3} \iiint \left[\frac{\hbar^2}{\mu\xi r_{rel}} - \frac{e^2}{4\pi\epsilon r_{rel}} - \frac{\hbar^2}{2\mu\xi^2}\right] e^{-\frac{2r_{rel}}{\xi}} r_{rel}^2 sin(\theta) dr d\theta d\phi \\ &= \frac{\hbar^2}{2\mu\xi^2} - \frac{e^2}{4\pi\epsilon\xi} \end{aligned} \tag{21}$$

(c) Minimizing the energy with respect to ξ:

$$\begin{aligned} 0 &= \frac{d\langle E\rangle}{d\xi} \\ &= \frac{e^2}{4\pi\epsilon\xi^2} - \frac{\hbar^2}{\mu\xi^3} \\ \rightarrow \xi &= \frac{4\pi\epsilon\hbar^2}{\mu e^2} \end{aligned} \tag{22}$$

which gives the corresponding energy:

$$\begin{aligned} \langle E\rangle &= \frac{\hbar^2}{2\mu}\frac{\mu^2 e^4}{(4\pi\epsilon)^2\hbar^4} - \frac{e^2}{4\pi\epsilon}\frac{\mu e^2}{4\pi\epsilon\hbar^2} \\ &= -\frac{\mu e^4}{32\pi^2\epsilon^2\hbar^2} \end{aligned} \tag{23}$$

(d) We see that the ξ found to minimize the energy is simply the Bohr radius, and the energy found is also identical to that found in (4.2).

4.5:

(a) The Bohr model of the hydrogen atom assumes that the electron revolves around the nuclei as a classical particle, but may only have angular momenta values of $n\hbar$.

(b) The electron's momentum is given by:

$$mvr = n\hbar \qquad n = 1, 2, \ldots \tag{24}$$

The centripetal force of the electron is simply the Coulomb attraction between the electron and proton:

$$\frac{e^2}{4\pi\epsilon r^2} = m\frac{v^2}{r} \tag{25}$$

Combining the above two equations and using $m = \mu$ (since the proton and electron masses are of the same order of magnitude):

$$\begin{aligned} \frac{e^2}{4\pi\epsilon r^2} &= \mu\frac{n^2\hbar^2}{\mu^2 r^3} \\ \rightarrow r_n &= \frac{4\pi\epsilon\hbar^2}{\mu e^2}n^2 \end{aligned} \tag{26}$$

The binding energy is given by:

$$\begin{aligned} E_n &= -\frac{e^2}{4\pi\epsilon r} + \frac{1}{2}\mu v^2 \\ &= -\frac{\mu e^4}{(4\pi\epsilon)^2\hbar^2}\frac{1}{n^2} + \frac{\mu e^4}{2(4\pi\epsilon)^2\hbar^2}\frac{1}{n^2} \\ &= -\frac{\mu e^4}{32\pi^2\epsilon^2\hbar^2}\frac{1}{n^2} \\ &= -\frac{R_X}{n^2} \quad \text{where} \quad R_X = \frac{\mu e^4}{32\pi^2\epsilon^2\hbar^2} \end{aligned} \tag{27}$$

(c) We see that the energy found in (4.2) is simply the ground state $n = 1$ energy.

(d) The peak of the probability distribution corresponds to the $n = 1$ orbit radius in the Bohr model.

4.6:

The electron-hole reduced mass in ZnS is given by:

$$\mu = \left(\frac{1}{.28m_0} + \frac{1}{.5m_0} \right)^{-1} = .1795m_0 \tag{28}$$

The exciton Rydberg energy is thus:

$$R_X = \frac{\mu R_H}{m_0 \epsilon_r^2} = .0391eV \tag{29}$$

The $n = 1$ and $n = 2$ exciton energies are thus:

$$E_1 = -.0391eV \quad \text{and} \quad E_2 = -.0098eV \tag{30}$$

The highest excited phonon energies at room temperature are approximately:

$$E_{max}^{\text{phonon}} \approx k_B(300K) = .0259eV \tag{31}$$

We thus see that the excited phonons do not have enough energy to ionize the $n = 1$ excitons, but can ionize the $n = 2$ excitons.

4.7:

We have the reduced mass in InP:

$$\mu = \left(\frac{1}{.077m_0} + \frac{1}{.2m_0} \right)^{-1} = .0556m_0 \tag{32}$$

The exciton Rydberg energy is thus:

$$R_X = \frac{\mu R_H}{m_0 \epsilon_r^2} = .0049eV \tag{33}$$

which gives the $n = 1$ and $n = 2$ exciton binding energies:

$$E_1 = -.0049eV \quad \text{and} \quad E_2 = -.0012eV \tag{34}$$

The corresponding wavelengths are:

$$\lambda_1 = \frac{hc}{E_g + E_1} = 873.8nm \quad \text{and} \quad \lambda_2 = \frac{hc}{E_g + E_2} = 871.5nm \tag{35}$$

which corresponds to a difference of $2.3nm$.

4.9:

We have the exciton Rydberg energy:

$$R_X = \frac{\mu R_H}{m_0 \epsilon_r^2} = 4.15meV \tag{36}$$

The $n = 1$ and $n = 2$ energies are given by:

$$E_1 = -4.15meV \quad \text{and} \quad E_2 = -1.04meV \tag{37}$$

The energy difference is $3.11meV$, which corresponds to a wavelength of $398.4\mu m$.

4.10:

For the ground state exciton, the electron-hole separation is the exciton Bohr radius a_X. We have the explicit expressions from (4.5):

$$a_X = r_1 = \frac{4\pi\epsilon\hbar^2}{\mu e^2} \qquad R_X = \frac{\mu e^4}{32\pi^2\epsilon^2\hbar^2} \tag{38}$$

According to the Bohr model, the electric field produced by the electron (hole) at the hole (electron) is given by:

$$\begin{aligned} |\mathcal{E}| &= \frac{1}{4\pi\epsilon}\frac{e}{a_X^2} \\ &= \frac{2R_X}{ea_X} \end{aligned} \tag{39}$$

4.11:

For germanium, the reduced mass is given by:

$$\mu = \left(\frac{1}{.038m_0} + \frac{1}{.1m_0}\right)^{-1} = .0275m_0 \tag{40}$$

The exciton Rydberg energy (ground state exciton energy) is thus:

$$R_X = \frac{\mu}{m_0\epsilon_r^2} R_H = 1.46meV \tag{41}$$

and the exciton Bohr radius (ground state exciton radius) is:

$$a_X = \frac{m_0\epsilon_r}{\mu} a_H = 30.78nm \tag{42}$$

The field magnitude at the electron and hole is:

$$|\mathcal{E}| = \frac{2R_X}{ea_X} = 94866.8\frac{V}{m} \tag{43}$$

For a bias voltage V_0, the field across the junction is given by:

$$|\mathcal{E}| = \frac{V_{bi} - V_0}{\ell_i} \tag{44}$$

The voltage at which the field equals the ionization field is:

$$V_0 = .74 - (94866.8)\left(2\times 10^{-6}\right) = .55V \tag{45}$$

4.12:

The exciton cyclotron energy is given by:

$$E_B = \hbar\frac{eB}{\mu} \tag{46}$$

Setting this equal to the exciton Rydberg energy:

$$\begin{aligned}\hbar\frac{eB}{\mu} &= \frac{\mu R_H}{m_0\epsilon_r^2}\\ \to B &= \frac{\mu^2 R_H}{\hbar e m_0 \epsilon_r^2}\end{aligned} \tag{47}$$

For GaAs with $\mu = 0.05m_0$ and $\epsilon_r = 12.8$, we find:

$$B = 1.799T \tag{48}$$

4.13:

For a vector potential of $\mathbf{A} = \frac{B}{2}\langle -y, x, 0\rangle$, the corresponding magnetic flux density is:

$$\begin{aligned}\mathbf{B} &= \nabla\times\mathbf{A}\\ &= \frac{B}{2}\left[-\frac{\partial A_y}{\partial z}\hat{\mathbf{i}} + \frac{\partial A_x}{\partial z}\hat{\mathbf{j}} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{\mathbf{k}}\right]\\ &= B\hat{\mathbf{k}}\end{aligned} \tag{49}$$

From equation (B.17), we have the form of the Hamiltonian:

$$\begin{aligned}\hat{H} &= \hat{H}_0 + \frac{e}{2m_0}\left(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}\right) + \frac{e^2(\mathbf{A}\cdot\mathbf{A})}{2m_0}\\ &= \hat{H}_0 + \frac{e^2B^2(x^2+y^2)}{8m_0}\end{aligned} \tag{50}$$

where we've noted in the Coulomb gauge the operators $\mathbf{p}$ and $\mathbf{A}$ commute:

$$\begin{aligned}[\mathbf{p},\mathbf{A}]f(\mathbf{r}) &= -i\hbar\nabla\cdot(\mathbf{A}f(\mathbf{r})) + i\hbar\mathbf{A}\cdot(\nabla f(\mathbf{r}))\\ &= -i\hbar(\nabla\cdot\mathbf{A})f(\mathbf{r}) - i\hbar\mathbf{A}\cdot\nabla f(\mathbf{r}) + i\hbar\mathbf{A}\cdot(\nabla f(\mathbf{r}))\\ &= -i\hbar(\nabla\cdot\mathbf{A})f(\mathbf{r})\\ &= 0\end{aligned} \tag{51}$$

which implies:

$$\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p} = 2\mathbf{p}\cdot\mathbf{A} = -2i\hbar\nabla\cdot\mathbf{A} = 0 \tag{52}$$

For excitons, the Hamiltonian above becomes:

$$\hat{H} = \hat{H}_0 + \frac{e^2 B^2}{8\mu}(x^2 + y^2) \tag{53}$$

The expectation value of the energy for an exciton in a spherically symmetric ($\ell = 0$) energy state n is thus:

$$\begin{aligned}\langle E\rangle &= \left\langle \psi_n \,\middle|\, \hat{H}_0 \,\middle|\, \psi_n \right\rangle + \frac{e^2 B^2}{8\mu}\left\langle \psi_n \,\middle|\, (x^2+y^2) \,\middle|\, \psi_n \right\rangle \\ &= E_0 + \frac{e^2 B^2}{8\mu}\left(\frac{2}{3}\left\langle r^2\right\rangle\right) \\ &= E_0 + \Delta E \quad \text{where} \quad \Delta E = \frac{e^2 B^2}{12\mu}\left\langle r^2 \right\rangle\end{aligned} \tag{54}$$

where we used the fact that the symmetry of the $\ell = 0$ state gives:

$$\left\langle x^2\right\rangle = \left\langle y^2\right\rangle = \left\langle z^2\right\rangle \quad \text{(for spherically symmetric states)} \tag{55}$$

4.14:

The Rydberg energy and the Bohr radius of excitons in GaAs are given by Table 4.1:

$$R_X = 4.2 \text{ meV} \qquad a_X = 13 \text{ nm} \tag{56}$$

The diamagnetic shift is thus given by:

$$\Delta E = \frac{e^2 B^2}{12\mu} a_X^2 = 0.05 \text{ meV} \tag{57}$$

This corresponds to a frequency shift 11.95 GHz. The wavelength shift must be calculated by including the Jacobian:

$$\begin{aligned}\frac{\Delta\lambda}{\Delta f} &= -\frac{c}{f^2} \\ \rightarrow \Delta\lambda &= -\Delta f \frac{c}{f^2}\end{aligned} \tag{58}$$

Given an exciton resonance at 1.515 eV (365.6 THz) under no magnetic field, we find a wavelength shift of:

$$\Delta\lambda = -(11.95 \times 10^9)\frac{c}{(365.6 \times 10^{12})^2} = 0.0268 \text{ nm} \tag{59}$$

4.15:

We first find the exciton reduced mass:

$$\mu = \left(\frac{1}{0.2m_0} + \frac{1}{1.2m_0}\right)^{-1} = 0.171 m_0 \tag{60}$$

The exciton Bohr radius in GaN is:

$$a_X = \frac{m_0 \epsilon_r}{\mu} a_H = 3.09nm \tag{61}$$

which gives the $n = 1$ and $n = 2$ exciton radii:

$$r_1 = 3.09nm \quad \text{and} \quad r_2 = 12.34nm \tag{62}$$

The Mott densities are approximately:

$$N_1 = \frac{3}{4\pi r_1^3} = 8.09 \times 10^{24} m^{-3} \quad \text{and} \quad N_2 = \frac{3}{4\pi r_2^3} = 1.27 \times 10^{23} m^{-1} \tag{63}$$

4.16:

The kinetic energy $\frac{3}{2}k_B T$ corresponds to a momentum of:

$$p = \sqrt{2mE} = \sqrt{3mk_B T} \tag{64}$$

which gives a deBroglie wavelength:

$$\lambda_{deB} = \frac{h}{p} = \frac{h}{\sqrt{3mk_B T}} \tag{65}$$

The BEC inter-particle separation is:

$$\begin{aligned} \frac{4}{3}\pi d^3 &= \frac{1}{2.612 \left(\frac{mk_B T_c}{2\pi\hbar^2}\right)^{\frac{3}{2}}} \\ \rightarrow d &= \left(\frac{3}{4(2.612)\pi}\right)^{\frac{1}{3}} \sqrt{\frac{2\pi\hbar^2}{mk_B T_c}} \end{aligned} \tag{66}$$

The ratio of λ_{deB} and d is given by:

$$\begin{aligned} \frac{d}{\lambda_{deB}} &= \left(\frac{3}{4(2.612)\pi}\right)^{\frac{1}{3}} \sqrt{\frac{h^2}{2\pi mk_B T_c}} \frac{\sqrt{3mk_B T_c}}{h} \\ &= \left(\frac{3}{4(2.612)\pi}\right)^{\frac{1}{3}} \sqrt{\frac{3}{2\pi}} \\ &= 0.31 \end{aligned} \tag{67}$$

4.17:

When discussing BEC condensation of excitons, it is the center of mass motion that matters. We thus consider the total exciton mass $M = 1.7m_0$ in equation 4.9. The BEC condensation temperature is thus:

$$T_c = \frac{2\pi\hbar^2}{Mk_B} \left(\frac{N}{2.612}\right)^{2/3} = 17.1 \text{ K} \tag{68}$$

1.18:

The electron-hole radius for the n^{th} exciton in NaI is given by:

$$r_n = \frac{m_0 \epsilon_r n^2}{\mu} a_H = n^2 \times 8.52 \text{ Å} \tag{69}$$

The $n = 1$ and $n = 2$ exciton radii are thus 8.52 Åand 3.41 nm. The $n = 1$ exciton radius is comparable to the unit cell size 0.65 nm, so the Wannier model is not valid. However, the $n = 2$ exciton radius is an order of magnitude larger than the unit cell size, so the Wannier model is valid.