

# 1 Single particle equations

The Hamiltonian for a single particle in a Harmonic oscillator and a magnetic field is given by:

$$H = \frac{1}{2m*} \left( \mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 + \frac{1}{2} m * \omega_0^2 (x^2 + y^2) + e\phi + \boldsymbol{\rho} \cdot \mathbf{B} \quad (1)$$

For minimum gauge the magnetic field is given by:

$$\mathbf{A} = \frac{B}{2} (-y, x, 0)$$

$$\mathbf{B} = B \mathbf{e}_z$$

- > A commutes with p and we have:

$$\begin{aligned} \left( \mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 &= p^2 + \frac{e}{c} (\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \frac{e^2}{c^2} A^2 \\ &= p^2 + \frac{Be}{c} (xp_y - yp_x) + \frac{B^2 e^2}{4c^2} (x^2 + y^2) \end{aligned}$$

- > Equation (1) becomes:

$$\begin{aligned} H &= \frac{1}{2m*} \left( p^2 + \frac{Be}{c} (xp_y - yp_x) + \frac{B^2 e^2}{4c^2} (x^2 + y^2) \right) \\ &\quad + \frac{1}{2} m * \omega_0^2 (x^2 + y^2) + e\phi + \boldsymbol{\rho} \cdot \mathbf{B} \\ &= \frac{-\hbar^2}{2m*} \left( \nabla^2 + i \frac{Be}{\hbar c} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right) \\ &\quad + \frac{1}{2} m * \left( \omega_0^2 + \frac{B^2 e^2}{4c^2 m^{*2}} \right) (x^2 + y^2) + e\phi + \boldsymbol{\rho} \cdot \mathbf{B} \end{aligned} \quad (2)$$

Using polar coordinates  $r, \theta$ :  $\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}$ ,  $x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} = \frac{\partial}{\partial \theta}$  and  $\omega^2 = \omega_0^2 + \frac{B^2 e^2}{4c^2 m^{*2}}$ ,  $H_S = e\phi + \boldsymbol{\rho} \cdot \mathbf{B}$  this equation becomes:

$$H = -\frac{\hbar^2}{2m*} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + i \frac{Be}{\hbar c} \frac{\partial}{\partial \theta} \right) + \frac{1}{2} m * \omega^2 r^2 + H_S \quad (3)$$

Separating variables:  $\Psi(r, \theta) = e^{im\theta} \psi(r) \chi(s_1)$ ,  $m = 0, \pm 1, \pm 2, \dots$ . The Schrodinger equation  $H\Psi = E\Psi \rightarrow$

$$\begin{aligned} & -\frac{\hbar^2}{2m*} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{m^2}{r^2} - \frac{Bem}{\hbar c} \right) \psi(r) + \frac{1}{2} m * \omega^2 r^2 \psi(r) = E\psi(r) \\ & \rightarrow \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{m^2}{r^2} - \frac{m^{*2} \omega^2}{\hbar^2} r^2 \right) \psi(r) \\ & \quad = - \left( E \frac{2m*}{\hbar^2} - \frac{Bem}{\hbar c} \right) \psi(r) \end{aligned} \quad (4)$$

$$(e\phi + \boldsymbol{\rho} \cdot \mathbf{B}) \chi(s_1) = E_S \chi(s_1) \quad (5)$$

Equation (4) can be written as:

$$\rightarrow A\psi(r) = \epsilon_m\psi(r) \quad (6)$$

Where A and  $\epsilon_m$  is given by:

$$A = \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{m^2}{r^2} - \frac{m^* \omega^2}{\hbar^2} r^2 \right) \quad (7)$$

$$\epsilon_m = \left( -E \frac{2m^*}{\hbar^2} + \frac{Bem}{\hbar c} \right) \quad (8)$$

## 2 Two-particle equations

$$H = \sum_{i=1}^2 \left[ \frac{1}{2m^*} \left( \mathbf{p}_i + \frac{e}{c} \mathbf{A}_i \right)^2 + \frac{1}{2} m^* \omega_0^2 r_i^2 + e\phi_i + \boldsymbol{\rho}_i \cdot \mathbf{B}_i \right] + \frac{e^2}{4\pi\epsilon\epsilon_0} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (9)$$

Using relative and center of mass coordinates defined as:

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2 & \mathbf{R} &= \frac{1}{2} (\mathbf{r}_1 + \mathbf{r}_2) \\ \mathbf{p} &= \frac{1}{2} (\mathbf{p}_1 - \mathbf{p}_2) & \mathbf{P} &= \mathbf{p}_1 + \mathbf{p}_2 \\ \mathbf{A}_r &= \frac{1}{2} (\mathbf{A}_1 - \mathbf{A}_2) & \mathbf{A}_R &= \mathbf{A}_1 + \mathbf{A}_2 \end{aligned}$$

Giving some relations:

$$\begin{aligned} r_1^2 + r_2^2 &= \frac{1}{2} (4R^2 + r^2) & p_1^2 + p_2^2 &= \frac{1}{2} (4p^2 + P^2) \\ \mathbf{p}_1 \cdot \mathbf{A}_1 + \mathbf{p}_2 \cdot \mathbf{A}_2 &= \frac{1}{2} (4\mathbf{p} \cdot \mathbf{A}_r + \mathbf{P} \cdot \mathbf{A}_R) \\ A_1^2 + A_2^2 &= 2A_r^2 + \frac{1}{2} A_R^2 \end{aligned}$$

Then H transforms:

$$\begin{aligned} H &= \frac{1}{2m^*} \left( p_1^2 + p_2^2 + \frac{2e}{c} (\mathbf{p}_1 \cdot \mathbf{A}_1 + \mathbf{p}_2 \cdot \mathbf{A}_2) + \frac{e^2}{c^2} (A_1^2 + A_2^2) \right) \\ &+ \frac{1}{2} m^* \omega_0^2 (r_1^2 + r_2^2) + \frac{e^2}{4\pi\epsilon\epsilon_0} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \sum_{i=1}^2 [e\phi_i + \boldsymbol{\rho}_i \cdot \mathbf{B}_i] \quad (10) \end{aligned}$$

$$H = \frac{1}{2m*} \left( 2p^2 + \frac{4e}{c} \mathbf{p} \cdot \mathbf{A}_r + \frac{2e^2}{c^2} A_r^2 + \frac{1}{2} P^2 + \frac{e}{c} \mathbf{P} \cdot \mathbf{A}_R + \frac{e^2}{2c^2} A_R^2 \right) + \frac{1}{2} m * \omega_0^2 \frac{1}{2} (4R^2 + r^2) + \frac{e^2}{4\pi\epsilon\epsilon_0} \frac{1}{r} + \sum_{i=1}^2 [e\phi_i + \boldsymbol{\rho}_i \cdot \mathbf{B}_i] \quad (11)$$

$$H = \frac{1}{m*} \left( \mathbf{p} + \frac{e}{c} \mathbf{A}_r \right) + \frac{1}{4} m * \omega_0^2 r^2 + \text{const.} \frac{1}{r} + \frac{1}{4m*} \left( \mathbf{P} + \frac{e}{c} \mathbf{A}_R \right) + m * \omega_0^2 R^2 + \sum_{i=1}^2 [e\phi_i + \boldsymbol{\rho}_i \cdot \mathbf{B}_i] \quad (12)$$

$$= H_r + H_R + H_S \quad (13)$$

Using separation of variables:  $\Psi(\mathbf{r}, \mathbf{R}, s_1, s_2) = \phi(\mathbf{r})\gamma(\mathbf{R})\chi(s_1, s_2)$

$$H\Psi = E\Psi \rightarrow \frac{H_r\phi(\mathbf{r})}{\phi(\mathbf{r})} + \frac{H_R\gamma(\mathbf{R})}{\gamma(\mathbf{R})} + \frac{H_S\chi(s_1, s_2)}{\chi(s_1, s_2)} = E \quad (14)$$

-> can be divided in separate equation which must each be a constant:

$$H_r\phi(\mathbf{r}) = E_r\phi(\mathbf{r}) \quad (15)$$

$$H_R\gamma(\mathbf{R}) = E_R\gamma(\mathbf{R}) \quad (16)$$

$$H_S\chi(s_1, s_2) = E_S\chi(s_1, s_2) \quad (17)$$

$$E = E_r + E_R + E_S \quad (18)$$

$$H_r = \frac{1}{m*} \left( \mathbf{p} + \frac{e}{c} \mathbf{A}_r \right) + \frac{1}{4} m * \omega_0^2 r^2 + \frac{e^2}{4\pi\epsilon\epsilon_0} \frac{1}{r} \quad (19)$$

$$H_R = \frac{1}{4m*} \left( \mathbf{P} + \frac{e}{c} \mathbf{A}_R \right) + m * \omega_0^2 R^2 \quad (20)$$

$$H_S = (\boldsymbol{\rho}_1 + \boldsymbol{\rho}_2) \cdot \mathbf{B} + e(\phi + \phi_2) \quad (21)$$

$$(22)$$

- > have two single particle equations that should be solved as in section 1. It is possible to set up a general equation to be solved.

### 3 General One-particle radial equation

The general equation become:

$$\left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{m^2}{r^2} - K \frac{1}{r} - \Omega^2 r^2 \right) \psi(r) = \epsilon_m \psi(r) \quad (23)$$

With constants given for each problem.

Single particle:  $\Omega^2 = \frac{m^* \omega^2}{\hbar^2}$ ,  $K = 0$ ,  $\epsilon_m = \frac{Bem}{\hbar c} - \frac{2m^* E}{\hbar^2}$ . This gives equation(4).

Relative:  $\Omega^2 = \frac{m^* \omega^2}{4\hbar^2}$ ,  $K = \frac{e^2}{4\pi\epsilon\epsilon_0}$ ,  $\epsilon_m = \frac{Bem}{\hbar c} - \frac{m^* E}{\hbar^2}$ .

COM:  $\Omega^2 = \frac{4m^* \omega^2}{\hbar^2}$ ,  $K = 0$ ,  $\epsilon_m = \frac{Bem}{\hbar c} - \frac{4m^* E}{\hbar^2}$ .

## 4 Finite difference equations

The general equation to be solved numerically is:

$$\left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{m^2}{r^2} - K \frac{1}{r} - \Omega^2 r^2 \right) \psi(r) = \epsilon_m \psi(r) \quad (24)$$

$$r_i = ih \quad u_i = \psi(r_i) \quad h = \frac{1}{N-1} \quad i = 0, 1, \dots, N-1$$

$N$  is the number of points.

For the derivatives we write:

$$\begin{aligned} \frac{\partial^2}{\partial r^2} u_i &\simeq \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} \\ \frac{\partial}{\partial r} u_i &\simeq \frac{u_{i+1} - u_{i-1}}{2h} \end{aligned}$$

Using this on (24) we get a non-symmetric tridiagonal matrix eigenvalue problem:

$$u_{i-1} \left( 1 - \frac{1}{2i} \right) + u_i \left( -2 - \frac{m^2}{i^2} - \Omega^2 i^2 h^4 - \frac{Kh}{i} \right) + u_{i+1} \left( 1 + \frac{1}{2i} \right) = \epsilon_m h^2 u_i \quad (25)$$