3D – n_e-el. QD

$$H = \frac{1}{2m^*}\sum_{i=1}^{n_e}(\vec{p}_i - e\vec{A}_i)^2 + \frac{1}{2}m^*\omega_0^2\sum_{i=1}^{n_e}\rho_i^2 + \frac{1}{2}m^*\omega_z^2\sum_{i=1}^{n_e}z_i^2 + \frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\sum_{i<j}^{1,n_e}\frac{1}{r_{ij}}$$

$$= \frac{1}{2m^*}\sum_{i=1}^{n_e}\vec{p}_i^{\,2} + \frac{1}{2}m^*\left(\Omega^2\sum_{i=1}^{n_e}\rho_i^2 + \omega_z^2\sum_{i=1}^{n_e}z_i^2\right) + \frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\sum_{i<j}^{1,n_e}\frac{1}{r_{ij}} - \omega_L L_z$$

$$\Omega^2 = \omega_0^2 + \omega_L^2$$

If $\tilde{\vec{r}}_i = \vec{r}_i/l_0$, $\tilde{\vec{p}}_i = \vec{p}_i l_0/\hbar$, $l_0 = (\hbar/m^*\omega_0)^{1/2}$

$$\mathcal{H} \equiv \frac{H}{\hbar\omega_0} = \frac{1}{2}\sum_{i=1}^{n_e}(\tilde{p}_i^2 + \tilde{\Omega}^2\tilde{\rho}_i^2 + \tilde{\omega}_z^2\tilde{z}_i^2) + k\sum_{i<j}^{1,n_e}\frac{1}{\tilde{r}_{ij}} - \tilde{\omega}_L M$$

Noninteracting case: $k=0$

$$\mathcal{H}_0 = \sum_{i=1}^{n_e} h_i,$$

$$h_i = \frac{1}{2}(\tilde{p}_i^2 + \tilde{\Omega}^2\tilde{\rho}_i^2 + \tilde{\omega}_z^2\tilde{z}_i^2) - \tilde{\omega}_L m_i$$

$$\epsilon_{n_{\rho i}, m_i, n_{zi}} = \tilde{\Omega}(2n_{\rho i} + |m_i| + 1) + \tilde{\omega}_z(n_{zi} + \tfrac{1}{2}) - \tilde{\omega}_L m_i$$

$$\psi_{n_{\rho i}, m_i, n_{zi}}(\tilde{\vec{r}}_i) = f_{n_{\rho i}, m_i}(\tilde{\rho}_i)\, g_{n_{zi}}(\tilde{z}_i)\, \frac{e^{im_i\varphi_i}}{\sqrt{2\pi}}$$

$$f_{n_{\rho i}, m_i}(\tilde{\rho}_i) = \sqrt{\frac{2\tilde{\Omega}\, n_{\rho i}!}{(n_{\rho i} + |m_i|)!}}\, x_i^{|m_i|} e^{-\frac{1}{2}x_i^2} L_{n_i}^{|m_i|}(x_i^2), \quad x_i = \tilde{\Omega}^{\frac{1}{2}}\tilde{\rho}_i,$$

$$g_{n_{zi}}(\tilde{z}_i) = \frac{(\tilde{\omega}_z/\pi)^{1/4}}{\sqrt{2^{n_{zi}} n_{zi}!}}\, e^{-\frac{1}{2}y_i^2} H_{n_{zi}}(y_i), \quad y_i = \tilde{\omega}_z^{\frac{1}{2}}\tilde{z}_i.$$

Then:

$$E_\alpha^{(0)} = \sum_{i=1}^{n_e}\epsilon_{n_{\rho i}, m_i}, \quad \Psi_\alpha^{(0)}(\tilde{r}_1, \dots, \tilde{r}_{n_e}) = \prod_{i=1}^{n_e}\psi_{n_{\rho i}, m_i, n_{zi}}(\tilde{r}_i),$$

$$\alpha = \{n_{\rho 1}, m_1, n_{z1}, \dots, n_{\rho n_e}, m_{n_e}, n_{z n_e}\}.$$

Full Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + k \sum_{i<j} \frac{1}{r_{ij}},$$

Schrödinger eq. $\mathcal{H}|\Psi\rangle = \mathcal{E}|\Psi\rangle$ in the eigenbasis of $\mathcal{H}_0$:

$$\langle\alpha|\mathcal{H}|\Psi\rangle = \mathcal{E}\langle\alpha|\Psi\rangle$$

$$\sum_\beta \underbrace{\langle\alpha|\mathcal{H}|\beta\rangle}_{\mathcal{H}_{\alpha\beta}}\underbrace{\langle\beta|\Psi\rangle}_{c_\beta} = \mathcal{E}\underbrace{\langle\alpha|\Psi\rangle}_{c_\alpha}$$

$$\sum_\beta \mathcal{H}_{\alpha\beta} c_\beta = c_\alpha, \qquad \mathcal{H}_{\alpha\beta} = \langle\alpha|\mathcal{H}|\beta\rangle$$

$$\mathcal{H}_{\alpha\beta} = \mathcal{E}^{(0)}_\alpha \delta_{\alpha\beta} + k \sum_{i<j}^{1,n_e} \langle\alpha|\tilde{r}_{ij}^{-1}|\beta\rangle$$

The interaction matrix elements:

$$\langle\alpha|\tilde{r}_{ij}^{-1}|\beta\rangle = \delta_{\alpha^*\beta^*} \underbrace{\langle n_{\rho i}, m_i, n_{zi}; n_{\rho j}, m_j, n_{zj}|\tilde{r}_{ij}^{-1}|n'_{\rho i}, m'_i, n'_{zi}; n'_{\rho j}, m'_j, n'_{zj}\rangle}$$

where $\alpha^* = \alpha/\{n_{\rho i}, m_i, n_{zi}; n_{\rho j}, m_j, n_{zj}\}$, $\beta^* = \beta/\{n'_{\rho i}, m'_i, n'_{zi}; n'_{\rho j}, m'_j, n'_{zj}\}$

and $|n_{\rho i}, m_i, n_{zi}; n_{\rho j}, m_j, n_{zj}\rangle = |\psi_{n_{\rho i}, m_i, n_{zi}}\rangle|\psi_{n_{\rho j}, m_j, n_{zj}}\rangle$.

Here:

$$\langle n_{\rho i}, m_i, n_{zi}; n_{\rho j}, m_j, n_{zj}|\tilde{r}_{ij}^{-1}|n'_{\rho i}, m'_i, n'_{zi}; n'_{\rho j}, m'_j, n'_{zj}\rangle =$$

$$= \int_0^{+\infty}\tilde{\rho}_i d\tilde{\rho}_i \int_0^{+\infty}\tilde{\rho}_j d\tilde{\rho}_j \int_0^{2\pi} d\varphi_i \int_0^{2\pi} d\varphi_j \int_{-\infty}^{+\infty} d\tilde{z}_i \int_{-\infty}^{+\infty} d\tilde{z}_j \, f_{n_{\rho i} m_i}(\tilde{\rho}_i) f_{n_{\rho j} m_j}(\tilde{\rho}_j) f_{n'_{\rho i} m'_i}(\tilde{\rho}_i) f_{n'_{\rho j} m'_j}(\tilde{\rho}_j)$$

$$g_{n_{zi}}(\tilde{z}_i)\, g_{n_{zj}}(\tilde{z}_j)\, g_{n'_{zi}}(\tilde{z}_i)\, g_{n'_{zj}}(\tilde{z}_j) \frac{e^{i(m'_i - m_i)\varphi_i}\, e^{i(m'_j - m_j)\varphi_j}}{4\pi^2(\tilde{\rho}_{ij}^2 + \tilde{z}_{ij}^2)^{1/2}}$$

$$\langle i, j | \tilde{r}_{ij}^{-1} | i', j' \rangle = \int_0^{\infty} \tilde{\rho}_i d\tilde{\rho}_i \int_0^{\infty} \tilde{\rho}_j d\tilde{\rho}_j \int_{-\infty}^{+\infty} d\tilde{z}_i \int_{-\infty}^{+\infty} d\tilde{z}_j \times$$

$$f_i(\tilde{\rho}_i) f_j(\tilde{\rho}_j) f_{i'}(\tilde{\rho}_i) f_{j'}(\tilde{\rho}_j) g_i(\tilde{z}_i) g_j(\tilde{z}_j) g_{i'}(\tilde{z}_i) g_{j'}(\tilde{z}_j) \cdot \langle m_i m_j | \tilde{r}_{ij}^{-1} | m_i' m_j' \rangle,$$

where:

$$\langle m_i m_j | \tilde{r}_{ij}^{-1} | m_i' m_j' \rangle = \frac{1}{4\pi^2} \int_0^{2\pi} d\varphi_i \int_0^{2\pi} d\varphi_j \frac{e^{i(m_i'-m_i)\varphi_i} e^{i(m_j'-m_j)\varphi_j}}{(\tilde{\rho}_{ij}^2 + \tilde{z}_{ij}^2)^{1/2}}$$

since:

$$\tilde{r}_{ij} = (\tilde{\rho}_{ij}^2 + \tilde{z}_{ij}^2)^{\frac{1}{2}} = \left[\tilde{\rho}_i^2 + \tilde{\rho}_j^2 - 2\tilde{\rho}_i \tilde{\rho}_j \cos(\varphi_i - \varphi_j) + (\tilde{z}_i - \tilde{z}_j)^2\right]^{1/2}$$

$$= \left[\tilde{r}_i^2 + \tilde{r}_j^2 - 2\tilde{z}_i \tilde{z}_j - 2\tilde{\rho}_i \tilde{\rho}_j \cos(\varphi_i - \varphi_j)\right]^{1/2}$$

$$= \sqrt{\tilde{r}_i^2 + \tilde{r}_j^2 - 2\tilde{z}_i \tilde{z}_j} \cdot \sqrt{1 - \frac{2\tilde{\rho}_i \tilde{\rho}_j}{\tilde{r}_i^2 + \tilde{r}_j^2 - 2\tilde{z}_i \tilde{z}_j} \cos(\varphi_i - \varphi_j)},$$

it is:

$$\langle m_i m_j | \tilde{r}_{ij}^{-1} | m_i' m_j' \rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{i(m_i' + m_j' - m_i - m_j)\varphi_j} d\varphi_j \times$$

$$\times \frac{1}{2\pi} \int_0^{2\pi} \frac{e^{i(m_i' - m_i)\varphi_{ij}'}}{r_{ij}'} d\varphi_{ij}$$

$$= \delta_{m_i + m_j, m_i' + m_j'} \cdot \frac{1}{2\pi} \int_0^{2\pi} \frac{e^{i(m_i' - m_i)\varphi_{ij}'}}{r_{ij}'} d\varphi_{ij}$$

$$= \frac{\delta_{m_i + m_j, m_i' + m_j'}}{(\tilde{r}_i^2 + \tilde{r}_j^2 - 2\tilde{z}_i \tilde{z}_j)^{1/2}} I_{m_i' - m_i}\left(\frac{2\tilde{\rho}_i \tilde{\rho}_j}{\tilde{r}_i^2 + \tilde{r}_j^2 - 2\tilde{z}_i \tilde{z}_j}\right),$$

where:

$$I_m(x) = \int_0^{2\pi} \frac{e^{im\varphi}}{\sqrt{1 - x\cos\varphi}} d\varphi.$$

$m_1, n_{e_1}, n_{z_1}, m_2, n_{e_2}, n_{z_2}$

a) $m_1, m_2 = -m, \dots, m$; $n_{e_1} = n_{e_2} = n_{z_1} = n_{z_2} = 0$

	m_1	m_2
$2m+1$	$-m$	$-m$
	$\vdots$	$\vdots$
	m	$-m$
	$\vdots$	$\vdots$
$2m+1$	$-m$	m
	$\vdots$	$\vdots$
	m	m

$(2m+1)^2$

$$\boxed{i = 1 + (m_1+m) + (2m+1)(m_2+m)}$$

b) $m_1, m_2 = -m, \dots, m$; $n_{e_1}, n_{e_2} = 0, \dots, n_{emax}$; $n_{z_1} = n_{z_2} = 0$

$$\boxed{i = 1 + (m_1+m) + (2m+1)(m_2+m) + (2m+1)^2 [n_{e_1} + (n_{emax}+1) n_{e_2}]}$$

	n_1	n_2
$n_{emax}+1$	0	0
	$\vdots$	$\vdots$
	n_{emax}	0
	$\vdots$	$\vdots$
$n_{emax}+1$	0	n_{emax}
	$\vdots$	$\vdots$
	n_{emax}	n_{emax}

$(n_{emax}+1)^2$

c) $m_1, m_2 = -m, \dots, m$; $n_{e_1}, n_{e_2} = 0, \dots, n_{emax}$; $n_{z_1}, n_{z_2} = 0, \dots, n_{zmax}$

$$i = 1 + (m_1+m) + (2m+1)(m_2+m) + (2m+1)^2 [n_{e_1} + (n_{emax}+1) n_{e_2}] +$$

$$+ (2m+1)^2 (n_{emax}+1)^2 \cdot [n_{z_1} + (n_{zmax}+1) n_{z_2}]$$