Excitons in nanostructures

Lection 1

<u>Excitons</u>

(*ground state of the crystal; bulk excitons, simplest case; center of mass motion and relative motion; bulk excitons in degenerate bands; quantization in a wide QW, in a narrow well, coulomb corrections; excitons in nanowires; excitons in quantum dots*)

Electron system of a crystal

(ground state)

$$\left[-\sum_i \frac{\hbar^2 \nabla_{r_i}^2}{2m_i} - \sum_i V(r_i) + \sum_{i<j} \frac{e^2}{\left|r_i - r_j\right|}\right] \psi(r_1, r_2, \ldots, r_N) = E\psi(r_1, r_2, \ldots, r_N)$$

For the ground state we can use determinant trial function:

$$\Psi(\mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(r_1) & . & . & . & \varphi_1(r_N) \\ . & . & . & . & . \\ \varphi_m(r_1) & . & . & . & \varphi_m(r_N) \\ . & . & . & . & . \\ \varphi_N(r_1) & . & . & . & \varphi_N(r_N) \end{vmatrix}$$

here $\varphi_m(r_1)$ single electron functions

can be used ether as Bloch functions
or as localized Wannier functions

With the same result

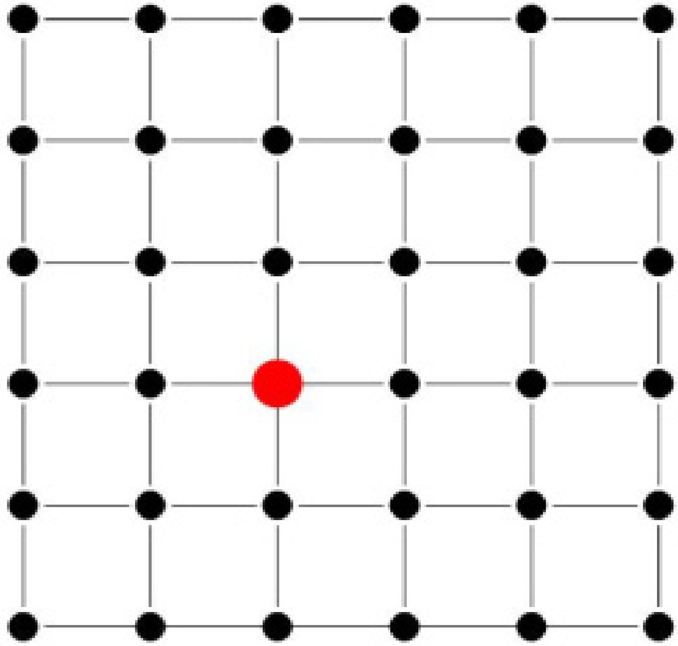
Bloch functions satisfied single electron equations

$$\left\{-\frac{\hbar^2}{2m_0}\nabla^2 + U_{eff}(\mathbf{r})\right\}\psi(\mathbf{r}) = \varepsilon\psi(\mathbf{r})$$

Wannier functions are a linear combination of the
Bloch functions

$$a_m(\mathbf{R}_n\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_k \mathrm{e}^{-i\mathbf{k}\mathbf{R}_n}\psi_m(\mathbf{k},\mathbf{r})$$

Excited state of the crystal



Because all position of the exited atom are equal,
this excitation can move free in the crystal

Excited state of crystal

(Frenkel exciton)

$$\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix} a_1(\mathbf{r}_1) & \ldots & \tilde{a}_m(\mathbf{r}_1) & \ldots & a_N(\mathbf{r}_1) \\ a_1(\mathbf{r}_2) & \ldots & \tilde{a}_m(\mathbf{r}_2) & \ldots & a_N(\mathbf{r}_2) \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ a_1(\mathbf{r}_N) & \ldots & \tilde{a}_m(\mathbf{r}_N) & \ldots & a_N(\mathbf{r}_N) \end{vmatrix}$$

$\tilde{a}_m(\mathbf{r}_1)$ wave function of the excited electron localized on the atom m *(Wannier or atomic functions)*

Excited state of crystal
(Wannier-Mott exciton)

$$\Psi_{\mathbf{k}_1,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\varphi_{1\mathbf{k}_1}(\mathbf{r}_1) & \ldots & \tilde{\varphi}_{m\mathbf{k}_2}(\mathbf{r}_1) & \ldots & \varphi_{N\mathbf{k}_1}(\mathbf{r}_1)\\ \varphi_{1\mathbf{k}_1}(\mathbf{r}_2) & \ldots & \tilde{\varphi}_{m\mathbf{k}_2}(\mathbf{r}_2) & \ldots & \varphi_{N\mathbf{k}_1}(\mathbf{r}_2)\\ \ldots & \ldots & \ldots & \ldots & \ldots\\ \ldots & \ldots & \ldots & \ldots & \ldots\\ \varphi_{1\mathbf{k}_1}(\mathbf{r}_N) & \ldots & \tilde{\varphi}_{m\mathbf{k}_2}(\mathbf{r}_N) & \ldots & \varphi_{N\mathbf{k}_1}(\mathbf{r}_N)\end{vmatrix}$$

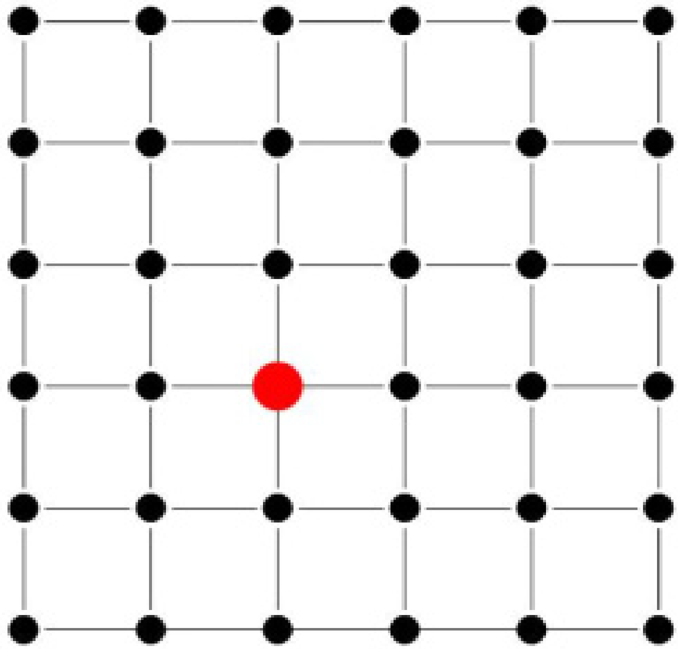
$\varphi_{lk}(\mathbf{r}_m)$ are single electron Bloch functions

$\varphi_N(\mathbf{r}_1)$ electron in the ground state

$\tilde{\varphi}_m(\mathbf{r}_2)$ electron in the excited state

Exciton

Because all position of the exited atom are equal,
we have to take a linear combination of such states



Exciton

Linear combination of the single electron determinants

$$\Psi_{exc}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n)=\sum_{\mathbf{k}_1,\mathbf{k}_2} f(\mathbf{k}_1,\mathbf{k}_2)\Psi_{\mathbf{k}_1,\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$$

$f(\mathbf{k}_1,\mathbf{k}_2)$ satisfy the equation

$$\left\{E-E_h(\mathbf{k}_1)+E_e(\mathbf{k}_2)+\sum_{\mathbf{k}'_1,\mathbf{k}_2'}(W(\mathbf{k}_1',\mathbf{k}_2';\mathbf{k}_1,\mathbf{k}_2)-W_{exch})\right\} f(\mathbf{k}_1,\mathbf{k}_2)=0$$

here

$$W(\mathbf{k}'_1,\mathbf{k}'_2;\mathbf{k}_1,\mathbf{k}_2)=-\int \varphi_{\mathbf{k}_1}^{*(1)}(\mathrm{r}_h)\,\varphi_{\mathbf{k}_2}^{*(2)}(\mathrm{r}_e)\frac{e^2}{r_{12}}\varphi_{\mathbf{k}_1}^{(1)}(\mathrm{r}_h)\,\varphi_{\mathbf{k}_2}^{(2)}(\mathrm{r}_e)\,d\tau_1 d\tau_2$$

$$W_{exch}(\mathbf{k}'_1,\mathbf{k}'_2;\mathbf{k}_1,\mathbf{k}_2)=\int \varphi_{\mathbf{k}_1}^{*(1)}(\mathrm{r}_h)\,\varphi_{\mathbf{k}_2}^{*(2)}(\mathrm{r}_e)\frac{e^2}{r_{12}}\varphi_{\mathbf{k}_2}^{(2)}(\mathrm{r}_e)\varphi_{\mathbf{k}_1}^{(1)}(\mathrm{r}_h)\,d\tau_1 d\tau_2$$

Exciton effective mass equation

For large distance between electron and hall, or for small **k** we obtain

$$\left[-\frac{\hbar^2\nabla_e^2}{2m_e^*}--\frac{\hbar^2\nabla_h^2}{2m_h^*}-\frac{e^2}{\varepsilon r_{eh}}\right]\Psi(\mathbf{r}_e,\mathbf{r}_h)=E\Psi(\mathbf{r}_e,\mathbf{r}_h)$$

<u>Center of mass and relative coordinates</u>

<u>Is it possible or not is not obvious</u>

$$\mathbf{R}=\alpha\,\mathbf{r}_e+\beta\,\mathbf{r}_h \quad \text{and} \quad \mathbf{r}=\mathbf{r}_e-\mathbf{r}_h$$

$$\nabla_e=(\nabla_{\mathbf{r}}+\alpha\nabla_{\mathbf{R}}) \qquad \nabla_h=(-\nabla_{\mathbf{r}}+\beta\nabla_{\mathbf{R}})$$

In bulk crystal it is possible and one can take

$$\alpha=\frac{m_e}{M} \qquad \beta=\frac{m_h}{M} \qquad M=m_e+m_h$$

In the center of mass **R** and relative **r** coordinates the exciton equations are

$$\left[-\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}} + H_0 + E\right]\Psi(\vec{R},\vec{r}) = 0$$

and

$$H_0 = -\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}} - \frac{e^2}{\kappa|\vec{r}|}$$

reduced mass $$\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}$$

solution $$\Psi_{ex}(\mathbf{r}_e,\mathbf{r}_h) = \phi(\mathbf{r})\, e^{i\mathbf{KR}}$$

For $\phi(\mathbf{r})$ equation

$$-\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}}\,\phi(\mathbf{r}) - \frac{e^2}{\varepsilon r}\phi(\mathbf{r}) = E_{ex}\,\phi(\mathbf{r})$$

The solution - <u>Hydrogen like spectrum</u>

$$R_n^B = \frac{n^2\varepsilon}{\mu}\frac{\hbar^2}{e^2}$$

Absorption peaks at:

$$\hbar\omega = E_g - \frac{\mu e^4}{2\hbar^2\varepsilon^2 n^2}$$

Hydrogen atom

energy $E = -\frac{me^2}{2\hbar^2 n^2}$

Wave functions $\varphi_{n,l,m}(r) = R_{n,l}(r) Y_l^m(\vartheta,\phi)$

$$R_{n,l} = -\frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{[(n+l)!]^2}}\, e^{-r/n}\left(\frac{2r}{n}\right)^l L_{n+1}^{2l+1}\left(\frac{2r}{n}\right)$$

$$Y_l^m(\vartheta,\phi) = (-1)^{m+|m|} i^l \left[\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\vartheta) e^{im\phi}$$

Several radial functions

$$R_{1,0} = 2e^{-r}$$

$$R_{2,0}(r) = \frac{1}{\sqrt{2}} e^{-r/2}\left(1 - \frac{r}{2}\right)$$

$$R_{2,1}(r) = \frac{1}{2\sqrt{6}} e^{-r/2} r$$

$$R_{3,0}(r) = \frac{2}{3\sqrt{3}} e^{-r/3}\left(1 - \frac{2}{3}r + \frac{2}{27}r^2\right)$$

$$R_{3,1}(r) = \frac{8}{27\sqrt{6}} e^{-r/3} r\left(1 - \frac{r}{6}\right)$$

$$R_{3,2}(r) = \frac{4}{81\sqrt{30}} e^{-r/3} r^2$$

Several spherical functions

$$Y_0^0 = \sqrt{\frac{1}{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\vartheta$$

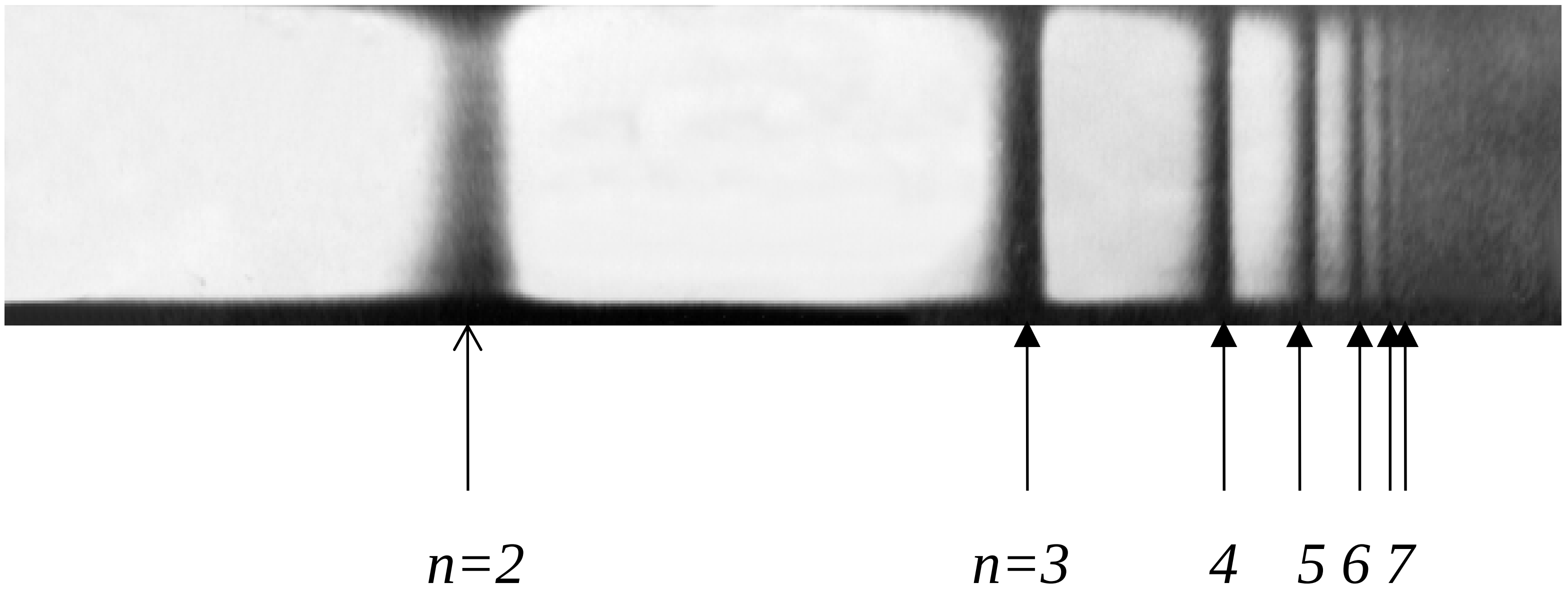
$$Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin\vartheta e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\vartheta - \frac{1}{2}\right)$$

$$Y_2^1 = \sqrt{\frac{15}{8\pi}} \sin\vartheta \cos\vartheta e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2\vartheta e^{2i\phi}$$

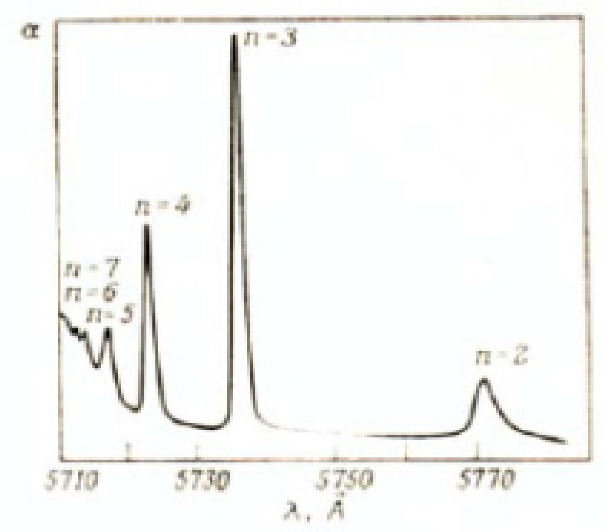
Exciton absorption of Cu2O



Sommerfeld factor

Arnold Johannes Wilhelm Sommerfeld

Line intensities in the discrete spectrum $\propto \left|\varphi_{n,0,0}(0)\right|^2 = \dfrac{1}{\pi a_B^3 n^3}$



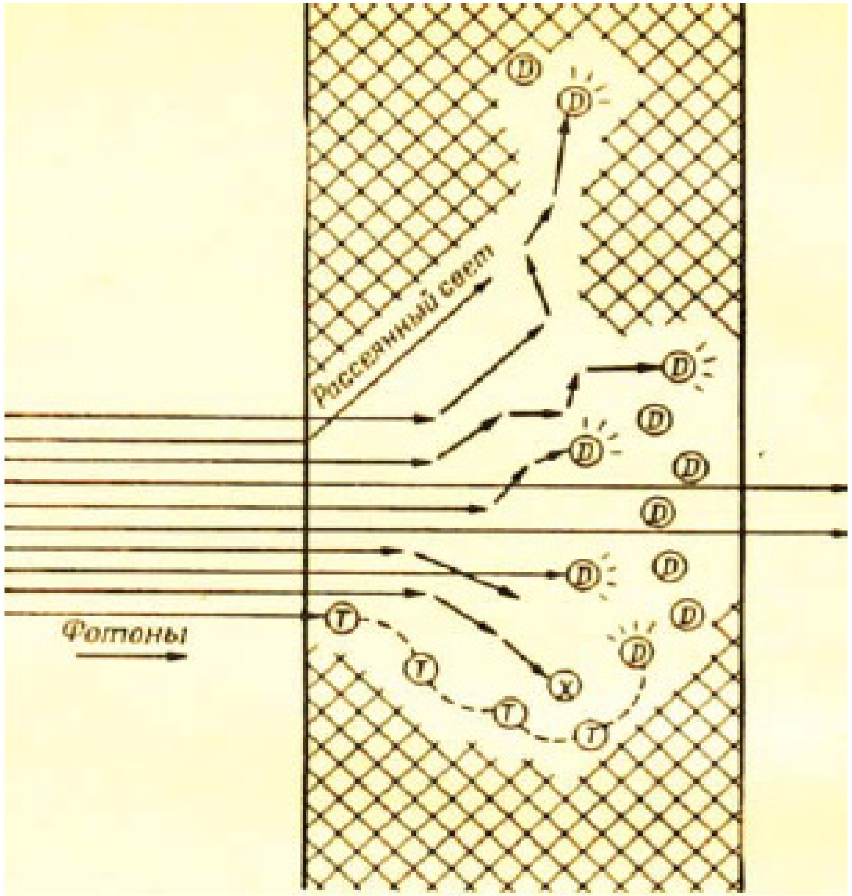
Exciton effect in the continuum spectrum

$$\frac{\left|\varphi(0)\right|^2}{\left|\varphi_k\right|^2} = \frac{\pi\beta \exp \pi\beta}{sh\pi\beta} \quad \text{here} \quad \beta = \frac{1}{ka_B}, \quad \varphi_k = \frac{1}{\sqrt{V}} e^{i\mathbf{kr}}$$

Due to the Sommerfeld factor exciton absorption is **3 times higher**

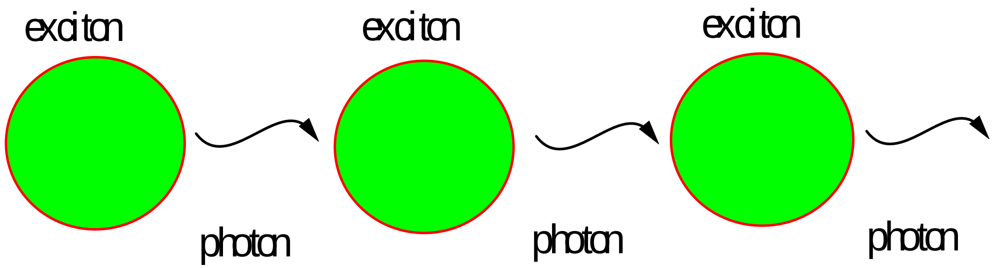
Exciton absorption

paradox: there is no absorption at all!



Real exciton is polariton

Chain of photon absorptions and emissions



No absorption in bulk crystal

Exciton is a photon in a crystal

(Lection_3)

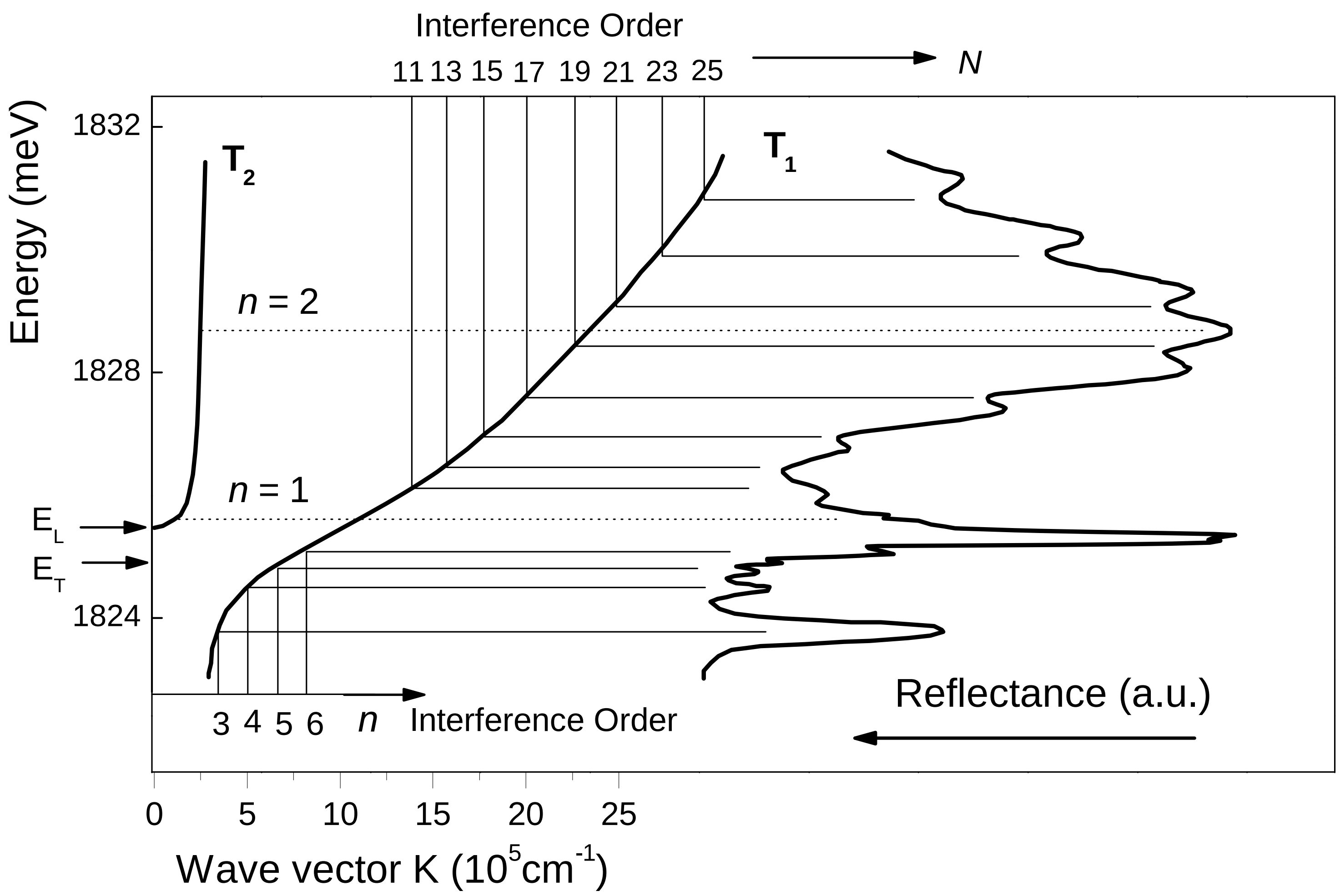
The central question:

Is it possible to consider the center of mass motion independently on the relative motion for the composite particle like exciton?

1). in bulk material?
2). in nanostructures?

Exciton in a bounded crystal

(first step to nanostructure)



Exciton in a bounded crystal

$$\left[-\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}} + H_0 + W(\mathbf{R},\mathbf{r}) + E\right]\Psi(\mathbf{R},\mathbf{r}) = 0 \qquad (EE)$$

$W(R,r)$ -the potential of the border of the crystal,

For this potential we can separate center of mass and relative motion

d - is the well thickness

$$W(R,r) = W(Z) = \begin{cases} 0 & \text{при } 0 < Z < d \\ \infty & \text{при } Z < 0 \text{ и } Z > d \end{cases}$$

The solution of the (EE) in infinite rectangular well is

$$\Psi(\mathbf{R},\mathbf{r}) = \frac{1}{\sqrt{S}} e^{i\mathbf{K}_{\|}\mathbf{R}_{\|}} F_N(\mathrm{Z})\,\varphi_{n,l,m}(\mathbf{r})$$

here $\mathbf{K}_{\|}$ and $\mathbf{R}_{\|}$ - are center of mass momentum and radius-vector

$\varphi_{n,l,m}(\mathbf{r})$ are hydrogen-like functions

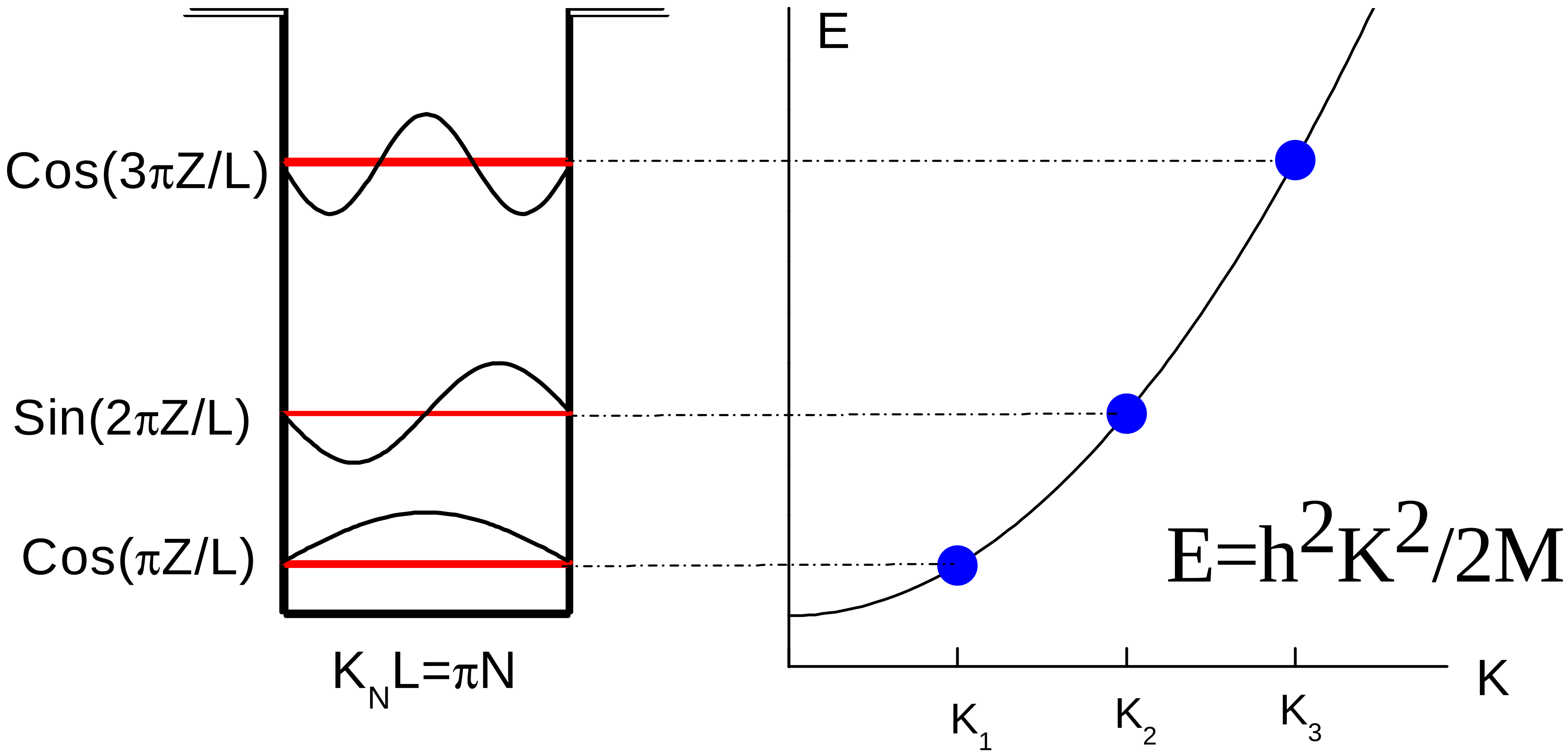
$F_N(\mathrm{Z})$ are eigenfunctions of the center of mass motion in the well $W(Z)$

$$F_N(\mathrm{Z}) = \sqrt{\frac{2}{d}} \begin{cases} \cos(N\pi \mathrm{Z}/d) & odd\ N \\ \sin(N\pi \mathrm{Z}/d) & even\ N \end{cases}$$

Energy spectrum for center of mass quantization

$$E_N = E_g - E_{n,l,m} + \frac{\hbar^2}{2M}\left[\left(\frac{\pi N}{d}\right)^2 + K_{\|}^2\right]$$

Exciton center of mass quantization



Odd and even states (*Lection 2 and 3*)

For arbitrary well necessary **adiabatic approximation**

(A.B.Migdal «*Qualitative Methods in Quantum Theory*»)

Adiabatic approximation

Electron – hole relative motion is FAST

Exciton center of mass motion is SLOW

Represent the wave function as $\Psi(R,r)=\sum_n \Phi_n(R)\phi_n(Z,r)$

$\phi_n(Z,r)$ wave functions of the fast subsystem, satisfy equation

$[H_0+V(Z,r)-E_n(Z)]\phi_n(Z,r)=0$ $\quad Z$ - is a parameter

Substituting $\Psi(R,r)$ into initial equation (*EE*) we get

$$\left[-\frac{\hbar^2}{2M}\nabla_R^2+E_n(Z)-E\right]\Phi_n(R)=\sum_m \Lambda_{nm}\Phi_m(R)$$

The way to generalize the adiabatic approximation

Operator of non adiabaticity

$$\Lambda_{nm} = \frac{\hbar^2}{M} \int \phi_n^* \frac{\partial}{\partial Z} \phi_m dr \frac{\partial}{\partial Z} + \frac{\hbar^2}{M} \int \phi_n^* \frac{\partial^2}{\partial Z^2} \phi_m dr$$

For adiabatic approximation $\Lambda_{nm} \equiv 0$

<u>This approximation works only for wide wells</u>

In this case the internal motion and center of mass motion are independent.

In a quantum well center of mass quantization for each state of internal motion.

Degenerate valence band

(Γ_8 band in cubic crystal)

Exciton Hamiltonian:

$$H = H_c(\mathbf{K}_e) - H_v(\mathbf{K}_h) - \frac{e^2}{\kappa|\vec{r}_e - \vec{r}_h|}$$

electrons

$$H_c(\mathbf{K}_e) = \hbar^2 \mathbf{K}_e^2 / 2m_e$$

here $\gamma = (2\gamma_2 + 3\gamma_3)/5$

$$\mathbf{K}_{e,h} = -i\nabla_{e,h}$$

holes

$$-H_v(\mathbf{K}_h) = \frac{\hbar^2}{2m_0}[(\gamma_1 + \frac{5}{2}\gamma)\mathbf{K}_h^2\mathbf{I} - 2\gamma(\vec{J}\mathbf{K}_h)^2]$$

$\gamma_1, \gamma_2, \gamma_3$ Luttinger parameters

Introduce relative and center of mass coordinates

$$\mathbf{r} = \mathbf{r}_e - \mathbf{r}_h$$

$$\mathbf{R} = \alpha\,\mathbf{r}_e + \beta\,\mathbf{r}_h$$

$\Rightarrow$

$$K_e = i(\nabla_{\mathbf{r}} + \alpha\nabla_{\mathbf{R}})$$

$$K_h = i(-\nabla_{\mathbf{r}} + \beta\nabla_{\mathbf{R}})$$

We can rewrite the exciton Hamiltonian as

$$H_{exc} = H_1(\vec{r}) + H_2(\vec{R}) + H_3(\vec{r},\vec{R})$$

here

Relative motion
$$H_1(r) = \frac{1}{2m_e}\mathbf{p}^2\mathbf{I} + \frac{1}{2m_0}(\gamma_1 + \frac{5}{2}\gamma)\mathbf{p}^2\mathbf{I} - \frac{\gamma}{m_0}(\mathbf{p}\vec{J})^2 - \frac{e^2}{\kappa|\vec{r}|}$$

Center of mass motion
$$H_2(R) = \frac{\hat{\alpha}^2}{2m_e}\hbar^2\mathbf{Q}^2\mathbf{I} + \frac{\hat{\beta}^2}{2m_0}(\gamma_1 + \frac{5}{2}\gamma)\hbar^2\mathbf{Q}^2\mathbf{I} - \frac{\gamma}{m_0}\hat{\beta}^2\hbar^2(\mathbf{Q}\vec{J})^2$$

Mixed term
$$H_3(r,R) = \frac{\hat{\alpha}\hbar}{m_e}(\mathbf{pQ})\mathbf{I} - \frac{\hat{\beta}\hbar}{m_0}(\gamma_1 + \frac{5}{2}\gamma)(\mathbf{pQ})\mathbf{I} + \frac{\hat{\beta}\hbar\gamma}{m_0}\{(\mathbf{p}\vec{J})(\mathbf{Q}\vec{J})\}$$

Is it possible to separate internal motion and center of mass motion?

In classical mechanics this is always possible

Separation of the center of mass motion and relative motion

Consider $\mathbf{Q}_x = \mathbf{Q}_y = 0 \quad \mathbf{Q}_z \neq 0$

We want for the Mixed term

$$\frac{\hat{\alpha}}{m_e}(\mathbf{p}_z\mathbf{Q}_z)\mathbf{I} - \frac{\hat{\beta}}{m_0}(\gamma_1 + \frac{5}{2}\gamma)(\mathbf{p}_z\mathbf{Q}_z)\mathbf{I} + \frac{2\hat{\beta}\gamma}{m_0}[(\mathbf{p}_z\mathbf{Q}_z)J_z^2] = 0$$

<u>The best that we can get</u>

$$\alpha_{hh,lh} = \frac{m_e}{m_e + m_{hh,lh}} \qquad \beta_{hh,lh} = \frac{m_{hh,lh}}{m_e + m_{hh.lh}}$$

$$m_{hh} = \frac{m_0}{(\gamma_1 - 2\gamma)} \qquad m_{lh} = \frac{m_0}{(\gamma_1 + 2\gamma)}$$

Exciton Hamiltonian

$$H = \frac{1}{2m_e}\mathbf{p}^2\mathbf{I} + \frac{1}{2m_0}(\gamma_1 + \frac{5}{2}\gamma)\mathbf{p}^2\mathbf{I} - \frac{\gamma}{m_0}(\mathbf{p}\vec{J})^2 + \frac{e^2}{\kappa|\vec{r}|} +$$

$$+\frac{\hat{\alpha}^2}{2m_e}\hbar^2\mathbf{Q}_z{}^2\mathbf{I} + \frac{\hat{\beta}^2}{2m_0}(\gamma_1 + \frac{5}{2}\gamma)\hbar^2\mathbf{Q}_z{}^2\mathbf{I} - \frac{\gamma}{m_0}\hat{\beta}^2\hbar^2(\mathbf{Q}_z\vec{J}_z)^2 +$$

$$\boxed{+\frac{\hat{\beta}\hbar\gamma}{m_0}\left(\mathbf{p}_x\{J_xJ_z\} + \mathbf{p}_y\{J_yJ_z\}\right)\mathbf{Q}_z}$$

conclusion

- For the internal motion we have two kind of excitons: heavy and light hole exciton
- For the center of mass motion we have also heavy and light excitons
- At small $\mathbf{Q}_z$ the internal motion and center of mass motion can not be separated

At small $\mathbf{Q}_z$ the exciton dispersion is essentially nonparabolic

$$\frac{\hat{\beta}\hbar\gamma}{m_0}\left(\mathbf{p}_x\{J_x J_z\}+\mathbf{p}_y\{J_y J_z\}\right)\mathbf{Q}_z \neq 0$$

(E.O.Kane «*Exciton dispersion in degenerate bands*» Phys.Rev. **B11**, 3850 (1975))

Exciton quantization in a narrow well

$$\left[\overbrace{-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2}+V(z_e)}^{\text{Electrons in the well}}\overbrace{-\frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial z_h^2}+V(z_h)}^{\text{Holes in the well}}\overbrace{-\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)}^{\text{Relative motion in the plane}}\overbrace{-\frac{e^2}{\kappa\sqrt{\rho^2+|z_e-z_h|^2}}}^{\text{Coulomb term}}\right]\Psi(\vec{r}_e,\vec{r}_h)=$$

$$\left(E-\frac{Q_\perp^2}{2M}\right)\Psi(\vec{r}_e,\vec{r}_h)$$

$Q_\perp^2 = Q_x^2 + Q_y^2$ Center of mass wave-vector in the plane of QW

$$\phi = arctg\left(\frac{x_e - x_h}{y_e - y_h}\right) \quad , \quad \rho - \sqrt{|x_e - x_h|^2 + |y_e - y_h|^2}$$

Solve in the limit $d \to 0$ In this case $\frac{e^2}{r} \approx \frac{e^2}{\rho}$

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = \frac{1}{\sqrt{S}} e^{i(Q_X X + Q_Y Y)} R^{2D}_{m,n}(\rho) \psi_{N_e}(z_e) \psi_{N_h}(z_h)$$

For quantization along z

$$\Psi_N(z) = \sqrt{\frac{2}{d}} \sin(\pi N z / d) \qquad E^{e,h}_N = \frac{\hbar^2 \pi^2 N^2}{2 m_{e,h} d^2}$$

For 2D exciton

$$R^{2D}_{n,m}(\rho) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} N_{n,|m|} \rho^{|m|} e^{-q_n \rho} L^{2|m|}_{n-|m|}(2 q_n \rho)$$

$$\varepsilon_{n,m} = -\frac{\mu e^4}{2\hbar^2 \kappa^2} \frac{1}{(n + |m| + 1/2)^2}$$

Finite QW width

adiabatic approximation

for $d << a$ ⇒ $\dfrac{\hbar^2}{m_e d^2} >> \dfrac{e^2}{\kappa a}$

one dimensional potential for hole

$$V_{N_e}^{m,n}(z_h) = \frac{e^2}{\kappa}\int d^2\rho\, dz \left|\varphi_{m,n}(\rho)\right|^2 \frac{2}{d}\sin^2\left(\frac{N_e \pi z_h}{d}\right)\left[\frac{1}{\rho} - \frac{1}{\sqrt{\rho^2 + \left|z - z_h\right|^2}}\right]$$

For $m=0$

$$V_{N_e}^{0,n}(z_h) = \frac{e^2}{\kappa}\left|\varphi_{0,n}(0)\right|^2 d\left[\frac{1}{4} + \left(\frac{z_h}{d} - \frac{1}{2}\right)^2 - \frac{1}{(N_e\pi)^2}\sin^2\left(\frac{N_e \pi z_h}{d}\right)\right]$$

Hole motion in the additional potential

$$\left\{-\frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial z_h^2}+\frac{e^2}{\kappa a}\frac{16}{(2n+1)^3}\frac{d}{a}\left[\frac{1}{4}+\left(\frac{z_h}{d}-\frac{1}{2}\right)^2-\frac{1}{(N_e\pi)^2}\sin^2\left(\frac{N_e\pi z_h}{d}\right)\right]-E_{N_h}^{N_e,n}\right\}\chi_{N_h}^{N_e,n}(z_h)=0$$

Two limit cases:

1) $\dfrac{\hbar^2}{m_h d^2} >> \left(\dfrac{d}{a}\right)\dfrac{e^2}{\kappa a}$ $\Rightarrow$ $\Delta E_{N_h}^{N_e,n}=\dfrac{e^2}{\kappa a}\dfrac{d}{a}\dfrac{16}{(2n+1)^2}\left[\dfrac{1}{3}-\dfrac{1}{2\pi^2}\left(\dfrac{1}{N_e^2}+\dfrac{1}{N_h^2}+\dfrac{\delta_{N_e,N_h}}{2N_e^2}\right)\right]$

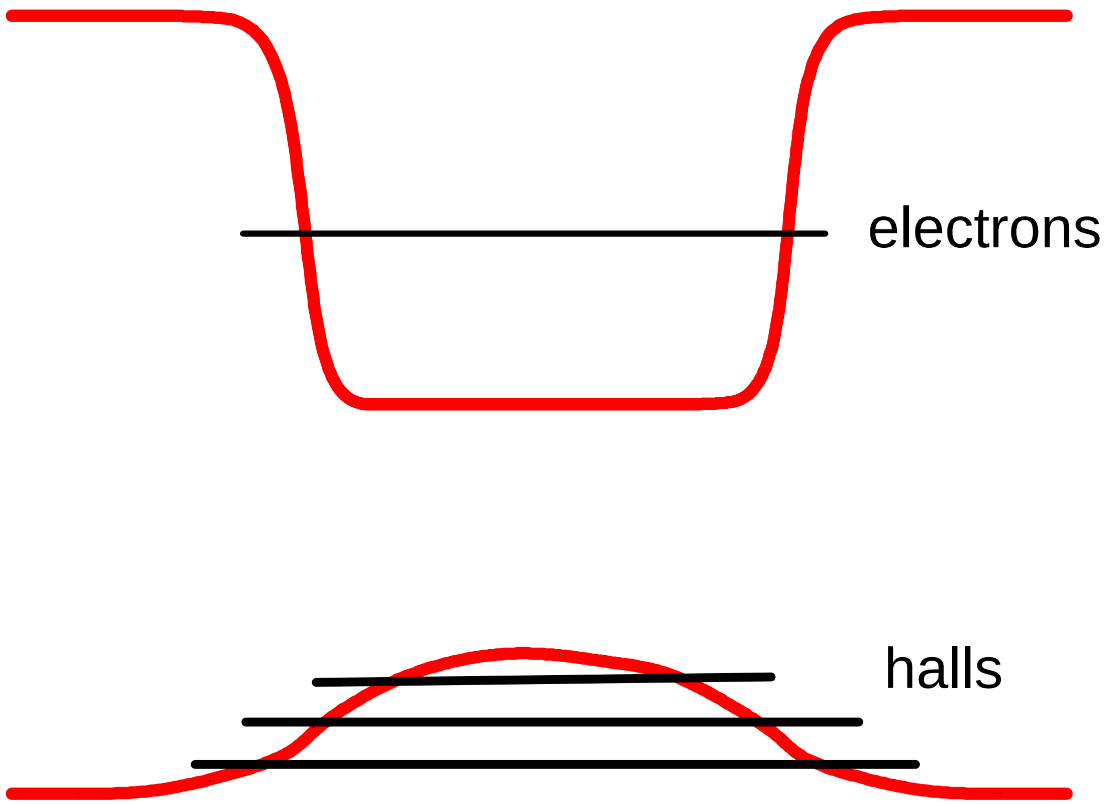
shift

2) $\dfrac{\hbar^2}{m_h d^2} << \left(\dfrac{d}{a}\right)\dfrac{e^2}{\kappa a}$ $\Rightarrow$ $E_{N_h}^{1,n}=\dfrac{e^2}{\kappa a}\dfrac{d}{a}\dfrac{16}{(2n+1)^2}\left(\dfrac{1}{4}-\dfrac{1}{\pi^2}\right)+\hbar\omega_h^n(N_h-\dfrac{1}{2})$

$$\hbar\omega_h^n=\sqrt{\frac{\hbar^2 e^2}{\kappa d}\frac{64}{a^2 m_h(2n+1)^3}}$$

Harmonic oscillator levels for hole

(Al.L.Efros Semicond. V.20, N0.7, p.1281 (1986))



Excitons in nanowires (NW)

Cylindrical wire

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}+V(\rho_e)+V(\rho_h)-\frac{\hbar^2}{2m_e}\left(\frac{1}{\rho_e}\frac{\partial}{\partial\rho_e}\rho_e\frac{\partial}{\partial\rho_e}+\frac{1}{\rho_e^{\,2}}\frac{\partial^2}{\partial\phi^2}\right)-\frac{\hbar^2}{2m_h}\left(\frac{1}{\rho_h}\frac{\partial}{\partial\rho_h}\rho_h\frac{\partial}{\partial\rho_h}+\frac{1}{\rho_h^{\,2}}\frac{\partial^2}{\partial\phi^2}\right)-\right.$$

$$\left.-\frac{e^2}{\kappa\sqrt{\left|\rho_e-\rho_h\right|^2+z^2}}\right)\Psi(\rho_e,\rho_h,\mathrm{z})=\left(E-\frac{Q_{\|}^2}{2M}\right)\Psi(\rho_e,\rho_h,\mathrm{z})$$

In the case of strong radial quantization, exciton wavefunction

$$\Psi_{QWW}^{exc}=\frac{\exp(iK_zZ)}{\sqrt{L}}f(z)\varphi_{e1}(\rho_e)\varphi_{h1}(\rho_h)u_c^0(\mathbf{r}_e)u_v^0(\mathbf{r}_h)$$

$\varphi_{e1}(\rho_e)$ and $\varphi_{h1}(\rho_h)$ Envelop functions for electron and hole

Boundary conditions:

$$\varphi_A = \varphi_B$$

$$\frac{1}{m_A}\left(\mathbf{N}\cdot\nabla\varphi\right)_A = \frac{1}{m_B}\left(\mathbf{N}\cdot\nabla\varphi\right)_B$$

$\mathbf{N}$ Normal vector to the NW surface

In cylindrical NW the projection of the angular momentum on z axis *M* is a good quantum number. For *M*=0

$$\varphi(\rho) = \begin{cases} C\,J_0(k\rho) & if\ \rho \le R \\ D\,K_0(\kappa\rho) & if\ \rho \ge R \end{cases}$$

Here *J* and *K* are Bessel functions, *R* is NW radius

$$k = \left(\frac{2m_A}{\hbar^2} - k_z^2\right)^{1/2} \qquad \kappa = \left(\frac{2m_B(\mathrm{V}-\mathrm{E})}{\hbar^2} + k_z^2\right)^{1/2}$$

The equations for D and C

$$D = CJ_0(kR)/K_0(\kappa R) \qquad \text{and} \qquad \frac{J_1(kR)K_0(\kappa R)}{J_0(kR)K_1(\kappa R)} = \frac{\kappa m_A}{k m_B}$$

For rectangular wire

$$E_{N_x,N_y,k} = \frac{\hbar^2}{2m_A}\left[\left(\frac{N_x\pi}{a_x}\right)^2 + \left(\frac{N_y\pi}{a_y}\right)^2 + k_z^2\right]$$

Exciton envelop function

$$-\frac{\hbar^2}{2\mu_{eh}}\frac{d^2 f(z)}{dz^2}+\tilde{V}_C(z)f(z)=E\ f(z)$$

Here $\tilde{V}_C(z)$ is effective coulomb potential

$$\tilde{V}_C(z)=-\frac{e^2}{\kappa}\int dx_e\, dy_e\, dx_h\, dy_h\,\frac{\varphi_{e1}^2(x_e,y_e)\,\varphi_{h1}^2(x_h,y_h)}{\sqrt{(x_e-x_h)^2+(y_e-y_h)^2+z}}$$

Trial function can be taken $f(\rho,\mathrm{z})\propto \exp\left(-\frac{\sqrt{\rho^2+z^2}}{a_z}\right)$

Excitons in quantum dots

Rectangular dot

$$\psi(\mathbf{r}) = \varphi_{N_x}(x, a_x)\,\varphi_{N_y}(y, a_y)\,\varphi_{N_z}(z, a_z)$$

$$E_e^{N_x, N_y, N_z} = \frac{\pi^2 \hbar^2}{2m_A}\left[\left(\frac{N_x}{a_x}\right)^2 + \left(\frac{N_y}{a_y}\right)^2 + \left(\frac{N_z}{a_z}\right)^2\right]$$

Spherical dot

In this case angular momentum conserves

For the ground state with zero angular momentum, <u>infinite barriers</u>

$$\psi(\mathbf{r}) = f(\mathbf{r})\left|s\right\rangle \qquad f(r) = \frac{1}{\sqrt{2\pi R}}\frac{\sin(\pi r / R)}{r}$$

$$E = \frac{\hbar^2 \pi^2}{2m_A R^2}$$

<u>Finite barriers</u>

$$f(r) = \frac{C}{r}\begin{cases} \sin kr & r \le R \\ e^{-\kappa(r-R)} \sin kR & r \ge R \end{cases}$$

Equation for the energy

$$1 - k\,R\,ctg(k\,R) = \frac{m_A}{m_B}(1 + \kappa R)$$

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