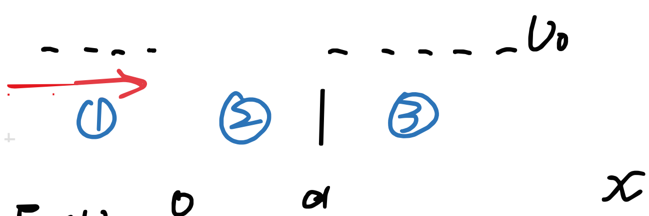
Extra

Quantum tunneling: Derive an expression for the transmission coefficient for a quantum particle ~~to~~ a rectangular potential barrier.



$E < U_0$

barrier: $x<0,\ x>a \longrightarrow U=0$

$0\le x\le a \longrightarrow U=U_0$

Schrödinger Equation (1-D): $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+U_0\psi(x)=E\psi(x)$

region ① $x<0$: $\psi_1(x)=Ae^{i\alpha x}+Be^{-i\alpha x}$; $\alpha=\frac{\sqrt{2mE}}{\hbar}$

region $0\le x\le a$: $\psi_2(x)=Ce^{\beta x}+De^{-\beta x}$; $\beta=\frac{\sqrt{2m(U_0-E)}}{\hbar}$

region $x>a$: $\psi_3(x)=A\xi e^{i\alpha x}$; $\alpha=\frac{\sqrt{2mE}}{\hbar}$

$\boxed{T=|\xi|^2}$

Boundary Condition

I @ $x=0$ $\psi_1(0)=\psi_2(0)$ $A+B=C+D$

$\left.\frac{d\psi_1}{dx}\right|_{x=0}=\left.\frac{d\psi_2}{dx}\right|_{x=0}\Rightarrow i\alpha(A-B)=\beta(C-D)$

$$\Rightarrow\begin{cases}2C=A+B+i\frac{\alpha}{\beta}(A-B)\\ 2D=A+B-\frac{i\alpha}{\beta}(A-B)\end{cases}\quad ①$$

II @ $x=a$ $\psi_3(0)=\psi_2(0)\Rightarrow A\xi e^{i\alpha a}=Ce^{\beta a}+De^{-\beta a}$

$\left.\frac{d\psi_3}{dx}\right|_{x=a}=\left.\frac{d\psi_2}{dx}\right|_{x=a}\Rightarrow$

$\frac{i\alpha}{\beta}A\xi e^{-i\alpha a}=Ce^{\beta a}-De^{-\beta a}$

$$\Rightarrow\begin{cases}2Ce^{\beta a}=(1+i\frac{\alpha}{\beta})e^{i\alpha a}A\xi\\ 2De^{-\beta a}=(1-i\frac{\alpha}{\beta})e^{i\alpha a}A\xi\end{cases}\quad ②$$

① ② $\Rightarrow$ $B=\frac{1+i\frac{\alpha}{\beta}}{1-i\frac{\alpha}{\beta}}\left(\xi e^{(i\alpha-\beta)a}-1\right)A$

$$\Rightarrow \xi=\frac{-4i\alpha/\beta}{(1-i\alpha/\beta)^2e^{(i\alpha+\beta)a}-(1+i\frac{\alpha}{\beta})e^{i(\alpha-\beta)a}}$$

$\xrightarrow{\text{if}}$ $\beta a \gg 1$ $\quad e^{-\beta a} \longrightarrow 0$

$$T = |\xi \xi^*| = \frac{16\alpha^2/\beta^2}{\left(1+\frac{\alpha^2}{\beta^2}\right)^2 e^{2\beta a}} = \frac{16\alpha^2\beta^2}{(\alpha^2+\beta^2)^2} e^{-2\beta a}$$

$$= \frac{16E(U_0-E)}{U_0^2} e^{-2\frac{\sqrt{2m(U_0-E)}}{\hbar} a}$$

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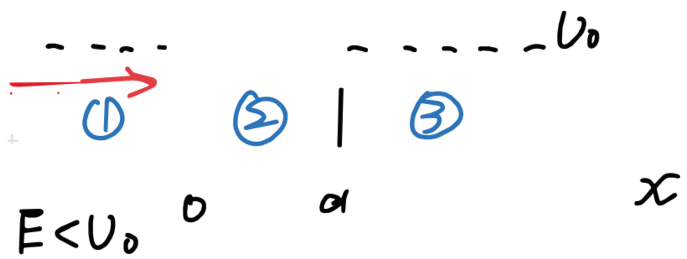


$$I = \frac{2}{L}\int \left(\frac{L}{n\pi}\right)^2 \xi \sin^2(\xi)\, d\xi$$

$$I = \frac{2L}{n^2\pi^2}\int_0^{n\pi} \xi \sin^2(\xi)\, d\xi = \frac{L}{n^2\pi^2}\int_0^{n\pi} \xi\,(1+\cos 2\xi)\, d\xi$$

$$= \frac{L}{n^2\pi^2}\left(\frac{1}{2}\xi^2\Big|_0^{n\pi} + \int_0^{n\pi} \xi \cos 2\xi\, d\xi\right)$$

$\eta = 2\xi$

$$= \frac{L}{n^2\pi^2}\left(\frac{1}{2}\xi^2\Big|_0^{n\pi} + \int_0^{n\pi} \frac{\eta}{2}\cos\eta\, \frac{d\eta}{2}\right)$$

$$= \frac{L}{n^2\pi^2}\left(\frac{1}{2}n^2\pi^2 + \frac{1}{4}\int_0^{n\pi} \underset{u}{\eta}\, \underset{dv}{\cos\eta\, d\eta}\right)$$

$$= \frac{L}{n^2\pi^2}\left(\frac{1}{2}n^2\pi^2 + \frac{1}{4}\left(\underbrace{\eta\sin\eta\Big|_0^{n\pi}}_{0} - \underbrace{\sin\eta\Big|_0^{n\pi}}_{0}\right)\right)$$

$$= \frac{L}{2}$$

II. $n \neq m$: 见初答案

$\boxed{\text{Extra:}}$

Derivation of Heisenberg uncertainty relation

Heisenberg uncertainty relation

$$\langle \Delta x \rangle \langle \Delta p \rangle \geq \frac{\hbar}{2}$$

$$\langle (\Delta x)^2 \rangle = \langle (x - \langle x \rangle)^2 \rangle$$

$$= \langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

$$2\langle x \rangle \langle x \rangle \qquad \langle \langle x \rangle^2 \rangle = \langle x \rangle^2$$

$$\langle (\Delta p_x)^2 \rangle = \langle (p_x - \langle p_x \rangle)^2 \rangle$$

$$= \langle p_x^2 - 2p_x \langle p_x \rangle + \langle p_x \rangle^2 \rangle = \langle p_x^2 \rangle - \langle p_x \rangle^2$$

chose coordinate system so that:

$$\langle x \rangle = 0, \quad \langle p_x \rangle = 0$$

$$I = \int \left| \alpha x \psi + \beta \frac{d\psi}{dx} \right|^2 dx \geq 0$$

$$\alpha, \beta \in \mathbb{R}$$

$$\left| \alpha x \psi + \beta \frac{d\psi}{dx} \right|^2 = \left(\alpha x \psi + \beta \frac{d\psi}{dx} \right) \left(\alpha x \psi^* + \beta \frac{d\psi^*}{dx} \right)$$

$$= \alpha^2 x^2 \psi \psi^* + \alpha\beta x \psi \frac{d\psi^*}{dx} + \alpha\beta x \frac{d\psi}{dx} \psi^* + \beta^2 \frac{d\psi}{dx} \frac{d\psi^*}{dx}$$

$$I = \alpha^2 \left(\int x^2 \psi \psi^* dx \right)$$

$$- \alpha\beta \left(\int - x \frac{d}{dx} (\psi \psi^*) \right) + \beta^2 \left(\int \left(\frac{d\psi^*}{dx} \right) \right.$$

$$\left. \left(\frac{d\psi}{dx} \right) dx \right)$$

$$\int x^2 \psi \psi^* dx = \langle x^2 \rangle$$

$$\int - x \frac{d}{dx} (\psi^* \psi) dx = - x (\underset{0}{\psi^* \psi}) \Big|_{-\infty}^{+\infty}$$

$$- \int \underset{1}{\psi^* \psi (- dx)}$$

$$\int \left(\frac{d}{dx} \psi^* \right) \left(\frac{d}{dx} \psi \right) dx = - \int \psi^* \left(\frac{d^2}{dx^2} \psi \right) dx$$

$$= \frac{1}{\hbar^2} \langle p_x^2 \rangle$$

$$p_x^2 = - \hbar^2 \frac{\partial}{\partial x^2} \quad p_x = -i\hbar \frac{\partial}{\partial x}$$

$$I = \alpha^2 \langle x^2 \rangle - \alpha\beta + \beta^2 \left(\hbar^{-2} \langle p_x \rangle \right) \geq 0$$

$$\xi = - \frac{\alpha}{\beta}$$

$$I = \langle x^2 \rangle \xi^2 + \xi + \hbar^{-2} \langle p_x^2 \rangle \geq 0$$

$$A\xi^2 + B\xi + C \geq 0$$

$$\Rightarrow \Delta = B^2 - 4AC < 0 \Rightarrow 1 - 4\langle x^2\rangle \frac{1}{\hbar^2}\langle p_x^2\rangle < 0$$

$$\Rightarrow \langle x^2\rangle\langle p_x^2\rangle \geq \frac{\hbar^2}{4}$$

方均根

$$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle \geq \frac{\hbar^2}{4}$$

$$\langle\Delta x\rangle\langle\Delta p_x\rangle \geq \frac{\hbar}{2}$$

Extra:

Assuming the hydrogen ground state wave function $\psi(r) = \frac{1}{\sqrt{\pi}} a_0^{-\frac{3}{2}} e^{-\frac{r}{a_0}}$. calculate the probability p that the electron is observed within a sphere of radius R centered at the position of the proton. Estimate the radius of which $p = \frac{1}{2}$ is observed!

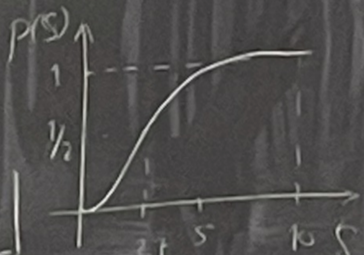
The probability dp to observe the electron in the volume element $d\theta$ is $dp = |\psi|^2 d\theta$

$$= |\psi|^2 r^2 \sin\theta \, d\theta \, d\varphi \, dr$$

$$P(R) = \frac{1}{\pi a_0^3} \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \underbrace{\int_0^{\pi} \sin\theta \, d\theta}_{2} \int_0^{R} r^2 e^{-\frac{2r}{a_0}} dr = \frac{4}{a_0^3} \int_0^{R} r^2 e^{-\frac{2r}{a_0}} dr$$

$$\varsigma = \frac{2r}{a_0} \; ; \; \varsigma_0 = \frac{2R}{a_0} \Rightarrow P(\varsigma_0) = \frac{1}{2} \int_0^{\varsigma_0} \varsigma^2 e^{-\varsigma} d\varsigma$$

by Parting integral: $P(\varsigma_0) = 1 - \left(1 + \varsigma_0 + \frac{\varsigma_0^2}{2}\right) e^{-\varsigma_0}$



$$\Rightarrow P(R) = 1 - \left[1 + \frac{2R}{a_0} + \frac{2R^2}{a_0^2}\right] e^{-\frac{2R}{a_0}} \; ; \quad P(0) = 0, \; P(R \to \infty) = 1$$

$p = \frac{1}{2} \Rightarrow \varsigma_0 = 2.68$ or $R = 1.34 a_0$ ※

$$= \frac{n!}{p^n}\int_0^\infty e^{-px}dx \longrightarrow \int_0^\infty e^{-px}dx$$

$$= \frac{n!}{p^n}\cdot\frac{1}{p} = \frac{n!}{p^{n+1}} \qquad = -\frac{1}{p}e^{-px}\Big|_0^\infty$$

$$= 0 + \frac{1}{p}$$

Extra

Regard the model case of anharmonic oscillator described by the model potential:

$$\hat{H}_{anharm} = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2x^2 + \alpha x^3 + \beta x^4\right]$$

Here, α and β are small Parameters. Basing on first order Pertubation theory anharmonic oscillator with respect to the harmonic oscillator

Solution:

The Perturbation $\hat{V} = \alpha x^3 + \beta x^4$

$$E_n = E_n^{(0)} + E_n^{(1)}$$

$$\frac{E_n^{(0)}}{m\omega_0^2} = (X)^2_{nn} = \sum X_{nj}X_{jn} = (X_n, X_{n-1})^2 + (X_n, X_{n+1})^2$$

$$= \frac{n\hbar}{2m\omega_0} + \frac{(n+1)\hbar}{2m\omega_0} = \frac{(2n+1)\hbar}{2m\omega_0}$$

$$X_{nm} = X_{mn}$$

$$(5.34) \longrightarrow E_n^{(1)} \simeq V_{nn}$$

$$E_n^{(1)} \simeq \alpha(x^3)_{nn} + \beta(x^4)_{nn} \qquad x^3 \text{ odd} \rightarrow \langle x^3\rangle_{nn} = 0$$

$$\langle x^4\rangle_{nn} = (x^2 x^2)_{nn} = \sum_j (x^2)_{nj}(x^2)_{jn} = \sum_l [(x^2)_{nl}]^2$$

$$(x^2)_{nl} = \sum_{j=n\pm1} x_{nj}x_{jl} = x_{n,n-1}x_{n-1,l} + x_{n,n+1}x_{n+1,l}$$

$$\Rightarrow l = n,\ n\mp 2$$

$$\langle x^4\rangle_{nn} = \sum_{l=n,n\pm2}[(x)^2_{nl}]^2 = [(x^2)_{nn}]^2 + [(x^2)_{n,n-2}]^2 + [(x^2)_{n,n+2}]^2$$

$$[(x^2)_{n,n-2}]^2 = [x_{n,n-1}\ x_{n-1,n-2}]^2$$

$$= \frac{n\hbar}{2m\omega_0} \times \frac{(n-1)\hbar}{2m\omega_0} = \frac{n(n-1)\hbar^2}{4m^2\omega_0^2}$$

$$[\langle x^2\rangle_{n,n+2}]^2 = [x_{n,n+1}\ x_{n+1,n+2}]^2$$

$$= \frac{(n+1)\hbar}{2m\omega_0} \times \frac{(n+2)\hbar}{2m\omega_0} = \frac{(n+1)(n+2)\hbar^2}{4m^2\omega_0^2}$$

$$[(x^2)_{n,n}]^2 = [\sum_{j=n\pm1} x_{nj}x_{jn}]^2 = [(x_{n,n-1})^2 + (x_{n,n+1})^2]^2$$

$$= \left(\frac{n\hbar + (n+1)\hbar}{2m\omega_0}\right)^2$$

$$= \frac{(2n+1)^2\hbar^2}{4m\omega_0^2}$$

$$\langle x^4\rangle_{nn} = \frac{\hbar^2}{4m\omega_0^2}\left[n(n-1) + (n+1)(n+2) + (2n+1)^2\right]$$

$$= \frac{3\hbar^2}{4m\omega_0^2}(2n^2+2n+1)$$

$$\longrightarrow E_n^{(1)} \simeq \beta\langle x^4\rangle_{nn} = \beta\frac{3\hbar^2}{4m^2\omega_0^2}(2n^2+2n+1)$$

$$E_n = E_n^{(0)} + E_n^{(1)} = \hbar\omega\left(n+\frac{1}{2}\right) + \beta\frac{3\hbar^2}{4m^2\omega_0^2}(2n^2+2n+1)$$

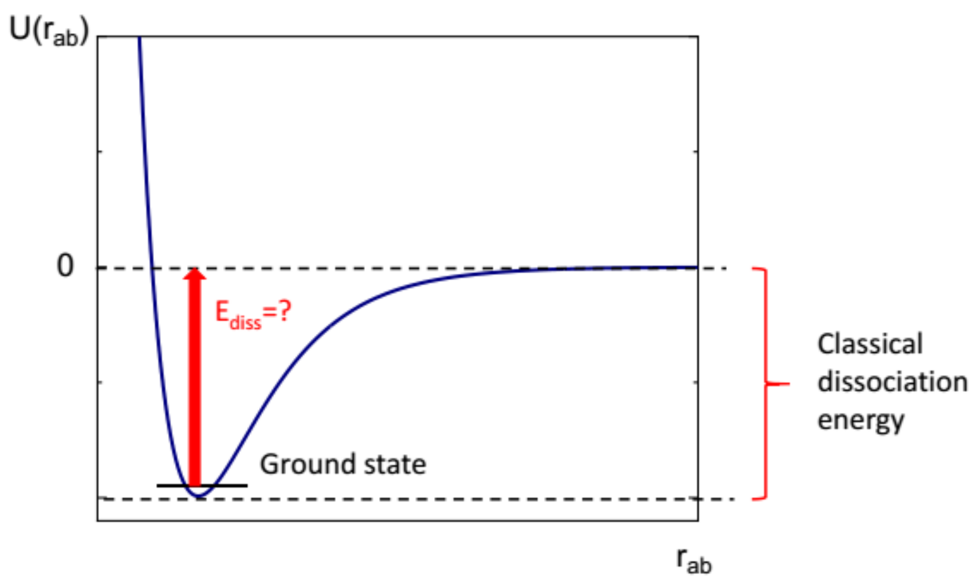
Extra:

Imagine that you have measured the absorption spectrum of a gas of (CF3)3CH molecules. Assume further, that you observe the fundamental transition wavenumber of the stretch vibration of the CH-group as $\nu_{1,0}$ = 2992cm^{-1}. You also register the transition wavenumber corresponding to the first overtone as $\nu_{2,0}$ = 5882cm^{-1}. From these data, assuming a Morse potential and neglecting any rotations, estimate the energy (in eV) necessary to dissociate a single CH group if the gas is held at room temperature.

Solution:

Provided that the gas is held at room temperature, we may assume that the thermal energy is much smaller than the energy necessary to excite a vibration of the CH-group. Hence, prior to the absorption process, the Morse-oscillator is certainly in its ground state. The energy necessary to dissociate the CH group starting from the vibrational ground state is different from the classical

dissociation energy D):



dissociation: $\epsilon_{vibr} = 0$

$$\epsilon_{diss} = -\epsilon_{vibr,\text{ground state}} = -hcG(v=0)$$

$$G(v) = -D_e + \nu_e\left(v+\frac{1}{2}\right) - \nu_e x_e\left(v+\frac{1}{2}\right)^2$$ (p. 143 script)

ν_e: charactristic wavenumber

$x_e = \frac{\nu_e}{4D_e} \ll 1$: degree of anharmonicity

ground state energy:

$$hcG(v=0) = \left[-D_e + \frac{\nu_e}{2} - \frac{\nu_e x_e}{4}\right]hc < 0$$

$$x_e = \frac{\nu_e}{4D_e} \Rightarrow G(v=0) = -D_e(1-x_e)^2$$

or $\epsilon_{diss} = hcD_e(1-x_e)^2$

D_e, x_e : ?

11.21:

$$\nu_{nm} = G(v=n) - G(v=m)$$

$$= \nu_e(n-m) - \nu_e x_e\left[\left(n+\frac{1}{2}\right)^2 - \left(m+\frac{1}{2}\right)^2\right]$$

$$= \nu_e(1-x_e)(n-m) - \nu_e x_e\left[n^2 - m^2\right]$$

$$m=0 \rightarrow \nu_{n,0} = \nu_e\left[(1-x_e)n - x_e n^2\right]$$

$$a \equiv \frac{\nu_{n_2,0}}{\nu_{n_1,0}} = \frac{\left[(1-x_e)n_2 - x_e n_2^2\right]}{\left[(1-x_e)n_1 - x_e n_1^2\right]}$$

$$\rightarrow x_e = \frac{a - n_2}{a(n_1+n_1^2) - (n_2+n_2^2)}$$

$$n_1 = 1,\ n_2 = 2\ ,\ a = \frac{\nu_{2,0}}{\nu_{1,0}} = \frac{5882}{2992} \approx 1.966$$

$$\rightarrow x_e \approx 0.0164$$

from $\nu_{n_1,0} = \nu_e\left[(1-x_e)n_1 - x_e n_1^2\right]$

$$\rightarrow \nu_e \approx 3093.5\ cm^{-1}$$

$$x_e = \frac{\nu_e}{4D_e} \rightarrow D_e \approx 47756.5\ cm^{-1}$$

$$\rightarrow E_{diss} = hcD_e(1-x_e)^2 \approx 5.66\ eV\ *$$

Extra:

Appendix to Chapt. 16: The Kronig-Penney model

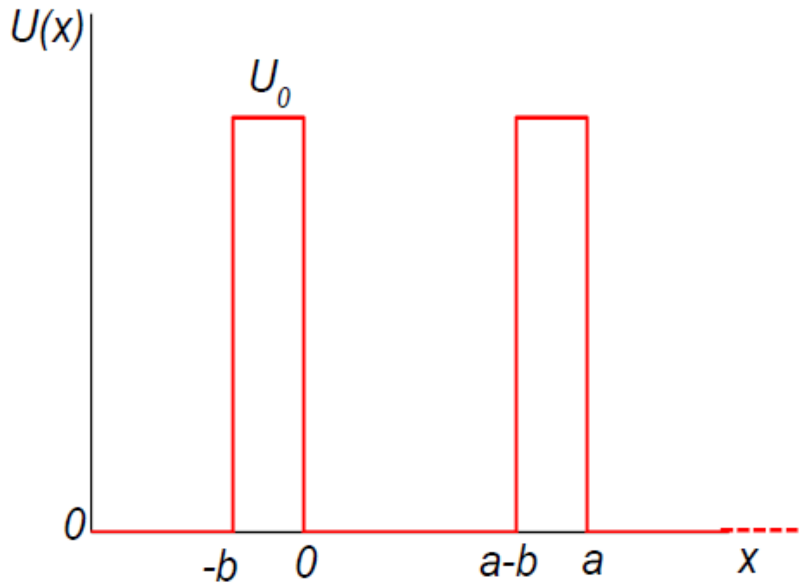


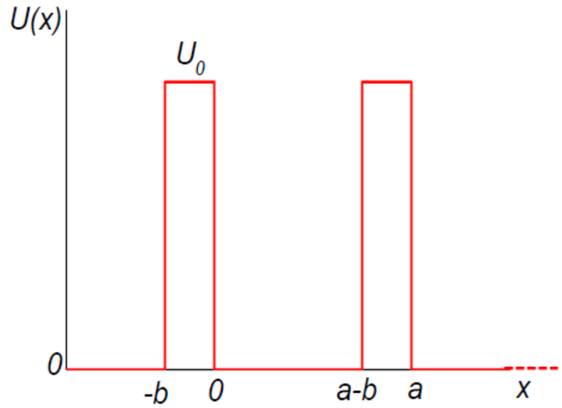
Fig. 16.5: Assumed model potential

Solution:

According to Tab. 4.1:

$$U=0:\ \psi_1(x)=Ae^{i\alpha x}+Be^{-i\alpha x};\ \alpha=\frac{\sqrt{2mE}}{\hbar}$$

$$U=U_0:\ \psi_2(x)=Ce^{\beta x}+De^{-\beta x};\ \beta=\frac{\sqrt{2m(U_0-E)}}{\hbar}$$



B.C. @ x = 0:

$$\psi_1(0)=\psi_2(0)\Rightarrow A+B=C+D$$

$$\left.\frac{d}{dx}\psi_1(x)\right|_{x=0}=\left.\frac{d}{dx}\psi_2(x)\right|_{x=0}\Rightarrow i\alpha(A-B)=\beta(C-D)$$

B.C. @ x = -b:

$$\psi_1(-b)=\psi_2(-b)\Rightarrow Ae^{-i\alpha b}+Be^{-i\alpha b}=Ce^{-\beta b}+De^{\beta b}$$

Periodic B.C.:

$$\psi_1(-b)=e^{-i\kappa a}\psi_1(a-b)\Rightarrow Ce^{-\beta b}+De^{\beta b}=e^{-i\kappa a}\left[Ae^{i\alpha(a-b)}+Be^{-i\alpha(a-b)}\right]$$

$$\beta\left(Ce^{-\beta b}-De^{\beta b}\right)=i\alpha e^{-i\kappa a}\left[Ae^{i\alpha(a-b)}-Be^{-i\alpha(a-b)}\right]$$

Four coefficients, four equations:

$$C+D=A+B$$

$$C-D=i\frac{\alpha}{\beta}(A-B)$$

$$Ce^{-\beta b}+De^{\beta b}=e^{-i\kappa a}\left[Ae^{i\alpha(a-b)}+Be^{-i\alpha(a-b)}\right]$$

$$Ce^{-\beta b}-De^{\beta b}=i\frac{\alpha}{\beta}e^{-i\kappa a}\left[Ae^{i\alpha(a-b)}-Be^{-i\alpha(a-b)}\right]$$

C and D are easily expressed through A+B and A-B. Substituting C and D into the last two equations:

$$(A+B)\left[\cosh\beta b-e^{-i\kappa a}\cos\alpha(a-b)\right]=i(A-B)\left[\frac{\alpha}{\beta}\sinh\,\beta b+e^{-i\kappa a}\sin\,\alpha(a-b)\right]$$

$$(A+B)\left[\sinh\,\beta b-\frac{\alpha}{\beta}e^{-i\kappa a}\sin\,\alpha(a-b)\right]=i(A-B)\frac{\alpha}{\beta}\left[\cosh\beta b-e^{-i\kappa a}\cos\alpha(a-b)\right]$$

Extra:

Wannier-Mott exciton in GaAs:

From M. Fox; "Optical Properties of Solids"

Example 4.1:

Part I.

Calculate the exciton Rydberg and Bohr radius for GaAs, which has $\epsilon_r = 12.8$, $m_e^* = 0.067m_0$ and $m_h^* = 0.2m_0$.

Solution:

SOM:

$$Ry = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{a_0} = \frac{e^4\mu}{8\varepsilon_0^2h^2} \approx 13.6eV \qquad (8.10)$$

$$E(n) = -\frac{\mu}{m_0}\frac{1}{\epsilon_r^2}\frac{R_H}{n^2} = -\frac{R_X}{n^2}$$

$$R_X = (\mu/m_0\epsilon_r^2)R_H$$

R_H = R_X

Part II.

GaAs has a cubic crystal structure with a unit cell size of 0.56 nm. Estimate the number of unit cells contained within the orbit of the $n = 1$ exciton. Hence justify the validity of assuming that the medium can be treated as a uniform dielectric in deriving eqns 4.1 and 4.2.

Solution:

We see from eqn 4.2 that the radius of the $n = 1$ exciton is equal to a_X. The volume occupied by this exciton is $\frac{4}{3}\pi a_X^3$ which is equal to 9.2×10^{-24} m^3. The volume of the cubic unit cell is equal to $(0.56 \text{ nm})^3 = 1.8 \times 10^{-28}$ m^3. Hence the exciton volume can contain 5×10^4 unit cells. Since this is a large number, the approximation of averaging the atomic structure to a uniform dielectric is justified.

SOM:

$$r_n = \frac{4\pi\varepsilon_0}{Ze^2\mu} n^2\hbar^2 = \frac{n^2}{Z}\frac{4\pi\varepsilon_0}{e^2\mu}\hbar^2 \equiv \frac{n^2}{Z}a_0 \tag{8.7}$$

With

$$a_0 = \frac{4\pi\varepsilon_0}{e^2\mu}\hbar^2 = \frac{\varepsilon_0}{e^2\pi\mu}h^2 \tag{8.8}$$

$$r_n = \frac{m_0}{\mu}\epsilon_r n^2 a_H = n^2 a_X$$

$$a_X = (m_0\epsilon_r/\mu)a_H$$

We first need to calculate the reduced electron–hole mass μ, which is given by eqn 3.22. With $m_e^* = 0.067m_0$, and $m_h^* = 0.2m_0$, we find

$$\mu = \left(\frac{1}{0.067m_0} + \frac{1}{0.2m_0}\right)^{-1} = 0.05m_0 .$$

We then insert this value of μ and $\epsilon_r = 12.8$ into eqns 4.1 and 4.2 to obtain:

$$R_X = \frac{0.05}{12.8^2} \times 13.6\,\text{eV} = 4.2\,\text{meV},$$

and

$$a_X = \frac{12.8}{0.05} \times 0.0529\,\text{nm} = 13\,\text{nm}.$$

Part III.

Estimate the highest temperature at which it will be possible to observe stable excitons in GaAs.

Solution:

The $n = 1$ exciton has the largest binding energy with a value of 4.2 meV. This is equal to $k_B T$ at 49 K. Therefore, we would not expect the excitons to be stable above $\sim$ 50 K.

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