2)

$$H = H_{cm} - \frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{\hbar^2}{2m_h}\nabla_h^2 - \frac{e^2}{\varepsilon r}$$

$$\vec{R} \equiv \frac{m_e\vec{r}_e + m_h\vec{r}_h}{m_e+m_h} \qquad \vec{r} = \vec{r}_e - \vec{r}_h$$

$$\frac{\partial}{\partial r_{e_x}} = \frac{\partial R_x}{\partial r_{e_x}}\frac{\partial}{\partial R_x} + \frac{\partial r_x}{\partial r_{e_x}}\frac{\partial}{\partial r_x} = \frac{m_e}{m_e+m_h}\frac{\partial}{\partial R_x} + \frac{\partial}{\partial r_x} \qquad \frac{\partial}{\partial r_{h_x}} = \frac{m_h}{m_e+m_h}\frac{\partial}{\partial R_x} - \frac{\partial}{\partial r_x}$$

$$\nabla_e^2 = \left(\frac{m_e}{m_e+m_h}\nabla_R + \nabla_r\right)^2 = \left(\frac{m_e}{m_e+m_h}\right)^2\nabla_R^2 + 2\frac{m_e}{m_e+m_h}\nabla_R\cdot\nabla_r + \nabla_r^2$$

$$\nabla_h^2 = \left(\frac{m_h}{m_e+m_h}\nabla_R - \nabla_r\right)^2 = \left(\frac{m_h}{m_e+m_h}\right)^2\nabla_R^2 - 2\frac{m_e}{m_e+m_h}\nabla_R\cdot\nabla_r + \nabla_r^2$$

$$-\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{\hbar^2}{2m_h}\nabla_h^2 = \left[\frac{m_e}{(m_e+m_h)^2}\nabla_R^2 + \cancel{\frac{1}{m_e+m_h}\nabla_R\cdot\nabla_r} + \frac{1}{m_e}\nabla_r^2 + \frac{m_h}{(m_e+m_h)}\nabla_R^2 - \cancel{\frac{1}{m_e+m_h}\nabla_R\cdot\nabla_r} + \frac{1}{m_h}\nabla_r^2\right]\left(-\frac{\hbar^2}{2m}\right)$$

$$= \underbrace{-\frac{\hbar^2}{2(m_e+m_h)}\nabla_R^2}_{-H_{cm}} - \frac{\hbar^2}{2}\underbrace{\left(\frac{1}{m_e}+\frac{1}{m_h}\right)}_{\frac{1}{\mu}}\nabla_r^2$$

$$= -H_{cm} - \frac{\hbar^2}{2\mu}\nabla_r^2$$

$$H = H_{cm} - H_{cm} - \frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{\varepsilon r} = -\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{\varepsilon r} \qquad H\Psi = E\Psi \qquad \Psi = \frac{1}{\sqrt{V_c}}\tilde{\phi}$$

envelope function

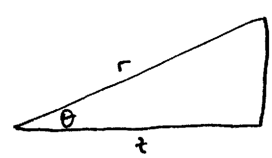
$$\left[\nabla_r^2 + \frac{2\mu E}{\hbar^2} + \frac{2\mu e^2}{\hbar^2\varepsilon}\frac{1}{r}\right]\tilde{\phi} = 0$$

In the asymptotic limit we expect solutions of the form

$$\tilde{\phi} \approx \underset{\substack{\uparrow \\ \text{plane wave}}}{e^{ikz}} + \underset{\substack{\uparrow \\ \text{spherical wave}}}{f(\theta)\frac{e^{ikr}}{r}} \qquad f(\theta) = \frac{e^2}{16\pi\varepsilon E\sin^2\frac{\theta}{2}} \quad \text{for Coulomb potential}$$

In parabolic coordinates

$$\xi = r - z = 2r\sin^2\frac{\theta}{2}$$
$$\eta = r + z = 2r\cos^2\frac{\theta}{2}$$



$$\tilde{\phi} = e^{ikz} + \frac{e^2}{16\pi\varepsilon E\sin^2\frac{\theta}{2}}\frac{e^{ikr}}{r} = e^{ikz}\left[1 + \frac{Ce^{ik\xi}}{\xi}\right] \qquad C \equiv \frac{e^2}{8\pi\varepsilon E}$$

$$\tilde{\phi} = e^{ikz}\,\Phi(\xi)$$

2 cont.) $\frac{\partial^2 \tilde{\Phi}}{\partial z^2} = -k^2 e^{ikz} \varphi + 2ik\, e^{ikz} \frac{d\varphi}{dz} + e^{ikz} \frac{d^2\varphi}{dz^2}$

$$\nabla^2 \tilde{\Phi} = e^{ikz}\left[-k^2\varphi + 2ik\frac{d\varphi}{dz} + \nabla^2\varphi\right]$$

$$0 = \nabla^2\tilde{\Phi} + \frac{2\mu E}{\hbar^2}\tilde{\Phi} + \frac{2\mu e^2}{\hbar^2 \varepsilon}\frac{1}{r}\tilde{\Phi} = e^{ikz}\left[\nabla^2\varphi + 2ik\frac{d\varphi}{dz} - \cancel{k^2\varphi} + \cancel{\frac{2\mu E}{\hbar^2}\varphi} + \frac{2\mu e^2}{\hbar^2\varepsilon}\frac{1}{r}\varphi\right] \qquad k^2 = \frac{2\mu E}{\hbar^2}$$

$$\nabla^2\varphi + 2ik\frac{d\varphi}{dz} + \frac{2\mu e^2}{\hbar^2\varepsilon}\frac{1}{r}\varphi = 0$$

In parabolic coordinates:

$$\nabla^2\varphi = \frac{4}{\xi+\eta}\frac{d}{d\xi}\left(\xi\frac{d\varphi}{d\xi}\right) = \frac{4}{\xi+\eta}\left[\frac{d\varphi}{d\xi} + \xi\frac{d^2\varphi}{d\xi^2}\right]$$

$$\frac{d\varphi}{dz} = -\frac{2\xi}{\xi+\eta}\frac{d\varphi}{d\xi} \qquad r = \tfrac{1}{2}(\xi+\eta)$$

$$\frac{4}{\xi+\eta}\left[\frac{d\varphi}{d\xi} + \xi\frac{d^2\varphi}{d\xi^2}\right] + 2ik\left(-\frac{2\xi}{\xi+\eta}\right)\frac{d\varphi}{d\xi} - \frac{2\mu e^2}{\hbar^2\varepsilon}\frac{2}{\xi+\eta}\varphi = 0$$

$$\xi\frac{d^2\varphi}{d\xi^2} + \left[1 - ik\xi\right]\frac{d\varphi}{d\xi} - \frac{\mu e^2}{\hbar^2\varepsilon}\varphi = 0$$

Kummer equation: $z\frac{d^2w}{dz^2} + (b-z)\frac{dw}{dz} - aw = 0$ has solution $w = {}_1F_1(a;b;z)$

So $\varphi = {}_1F_1\left(-\frac{i\mu e^2}{\varepsilon k\hbar^2}; 1; ik\xi\right)$ up to a normalization constant

$$\tilde{\Phi} = \underset{\substack{\uparrow \\ \text{norm}}}{B}\, e^{ikz}\, {}_1F_1\left(-\frac{i\mu e^2}{\varepsilon k\hbar^2}; 1; ik\xi\right)$$

Solve for B using mathematica or similar program

$$B = \exp\left(-\frac{\pi\mu e^2}{2\hbar^2\varepsilon k}\right)\Gamma\left(1 + i\frac{\mu e^2}{\hbar^2\varepsilon k}\right) \qquad \alpha^2 \equiv \frac{\mu e^4}{2\hbar^2\varepsilon^2 E} \qquad k = \frac{\sqrt{2\mu E}}{\hbar}$$

$$B = e^{+\frac{\pi\alpha}{2}}\Gamma(1+i\alpha)$$

$$|\Psi|^2_{r=0} = \frac{1}{V_c}|\tilde{\Phi}|^2_{r=0} = \frac{1}{V_c}e^{+\frac{\pi\alpha}{2}\cdot 2}|\Gamma(1+i\alpha)|^2\,|\cancel{{}_1F_1(-\alpha,1,0)}^{\,1}|^2 = \frac{e^{+\pi\alpha}|\Gamma(1+i\alpha)|^2}{V_c}$$

$$|\Gamma(1+i\alpha)|^2 = \frac{\pi\alpha}{\sinh(\pi\alpha)} \Rightarrow |\Psi|^2_{r=0} = \frac{e^{+\pi\alpha}\pi\alpha}{\sinh(\pi\alpha)}$$

The expectation value near r=0 is much larger than ignoring Coulomb interactions, giving a larger absorption.

3. Plot the exciton-polariton transverse and longitudinal branches for GaAs and PbI_2. (only 1s states)
lead di-iodide.

from lecture notes. and literature.

PRB, 38 7874 (1998).
W.J. Rappel
Exciton-polariton picture of the free-exciton lifetime in GaAs.

the dielectric response of GaAs as a function of wave number $\vec{k}$ and energy E is described as:

$$\epsilon(k, E) = \epsilon_b + \frac{4\pi\beta E_T^2(k=0)}{E_T^2(k) - E^2} = \epsilon_b + \frac{4\pi\beta E_0^2}{E_T^2 - E^2} \quad (1)$$

where. ϵ_b is the background dielectric constant (w/o considering excitons).

$E_T(k)$ is the dispersion of the exciton

$E_T(k) = E_0 + \hbar^2 k^2/2m^*$, m^* is effective mass of the exciton.

β is the polarizability of the exciton

→ For transverse mode. $\epsilon(\vec{k}, E) = \dfrac{(\hbar c \vec{k})^2}{E^2}$. (2)

$$(1), (2) \Rightarrow \frac{(\hbar c \vec{k})^2}{E^2} = \epsilon_b + \frac{4\pi\beta E_0^2}{E_T^2 - E^2}$$

$$\epsilon_b E^4 - (\epsilon_b E_T^2 + 4\pi\beta E_0 + \hbar^2 c^2 k^2) E^2 + \hbar^2 c^2 k^2 E_T^2 = 0$$

$$\Rightarrow E_\pm^2 = \frac{(\epsilon_b E_T^2 + 4\pi\beta E_0^2 + \hbar^2 c^2 k^2) \pm \sqrt{(\epsilon_b E_T^2 + 4\pi\beta E_0^2 + \hbar^2 c^2 k^2)^2 - 4\epsilon_b \hbar^2 c^2 k^2 E_T^2}}{2\epsilon_b} \quad (3)$$

→ For longitudinal mode: $\epsilon(\vec{k}, \vec{E}) = 0$. (4)

$$(1), (4) \Rightarrow 0 = \epsilon_b + \frac{4\pi\beta E_0^2}{E_T^2 - E^2}$$

$$\Rightarrow E = \sqrt{\frac{4\pi\beta E_0^2}{\epsilon_b} + E_T^2}$$

For GaAs. (PRB)

$m^* = 0.6\, m_e$

$\epsilon_b = 12.56.$

$$E_T = 1.5151 + \frac{\hbar^2 k^2}{2(0.6\, m_e)}$$

$\beta = 1.06 \times 10^{-4}.$

For PbI_2 (Polariton Relaxation and Bound Exciton Formation in PbI_2 Studied by Excitation spectra. JPSP, 63, 785 (1994))

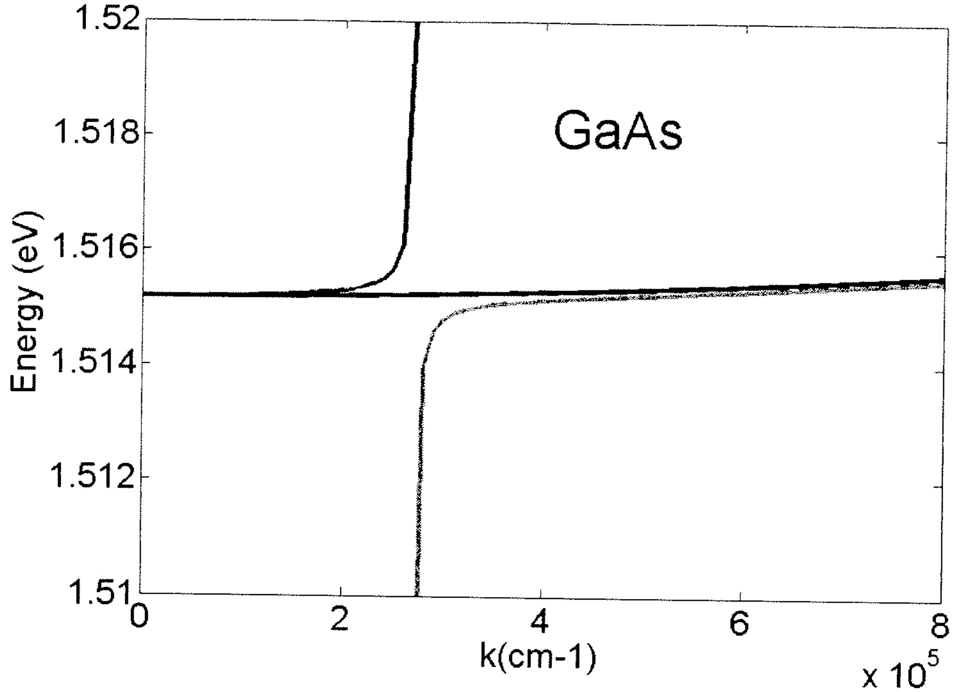
$m^* = 0.6\, m_e$

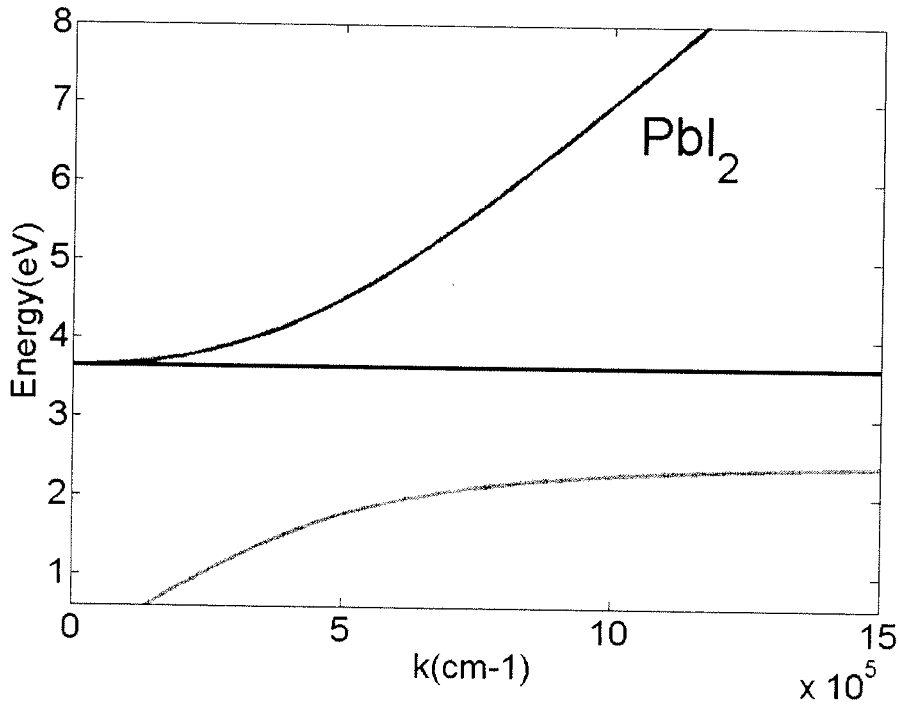
$\epsilon_b = 9.6.$

$$E_T = 2.49 + \frac{\hbar^2 k^2}{2 m_e}$$

$\beta = 0.868.$ (Physical Review. 76, 1215, 1949)

Problem 3


GaAs
Energy (eV)
1.52
1.518
1.516
1.514
1.512
1.51
0
2
4
6
8
k(cm-1)
x 10^5


PbI2
Energy(eV)
8
7
6
5
4
3
2
1
0
5
10
15
k(cm-1)
x 10^5

5. Absorption spectrum of poly (p-phenylene vinylene) (PPV)

H-R (Huang - Rhys) Model 80 K & 300 K.

absorption

$$\alpha = \sum_n \frac{|\langle 1|\mu_e|\rangle^{2}|^2 |\langle n_u|0_G\rangle|^2}{[\omega^2 - (E_G + n\hbar\underbrace{\Omega}_{\text{phonon freq.}})^2]^2 + \omega^2\Gamma_n^2}.$$

$$\text{where } |\langle n_u|0_G\rangle|^2 = e^{-s^2/2}\frac{(s^2/2)^n}{n!} \quad \text{(H-R factor)}.$$

For 80 K.

$$\frac{I(n=4)}{I(n=3)} = \frac{1}{2}$$

$$\frac{e^{-s^2/2}(s^2/2)^4}{4!} = \frac{e^{-s^2/2}(s^2/2)^3}{3!} \times \frac{1}{2}$$

$$\Rightarrow \frac{s^2}{2} = 2 \quad \Rightarrow S = 2$$

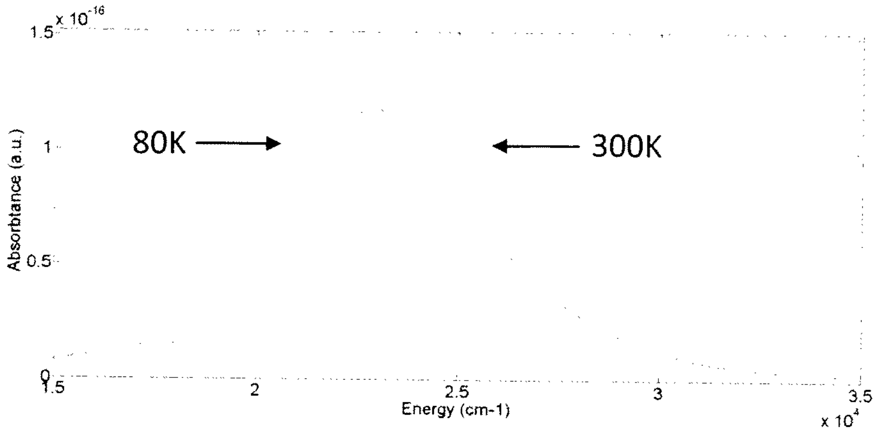
for 300 K

$$\frac{I(n=4)}{I(n=2)} = \frac{1}{2}$$

$$\frac{e^{-s^2/2}(s^2/2)^4}{4!} = \frac{e^{-s^2/2}(s^2/2)^2}{2!} \times \frac{1}{2}$$

$$\Rightarrow \left(\frac{s^2}{2}\right)^2 = 6. \quad \Rightarrow S = 2.2$$

Problem 5




```
At 80K
s=2;Eg=20000;Omg=1700;Gamma=2700;
```

At 300K

```
s=2.2;Eg=20500;Omg=1700;Gamma=2700;
```