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EE 381: Electronic Properties of Materials
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# Homework 5

## Problem 1

Infinitely deep 1D quantum well of width $L = 2$ nm $= 2 \times 10^{-9}$ m. Levels $m = 1, 2, 3$ are completely filled, level $m \geq 4$ are empty. Electron mass is the free electron mass $m_e$.

We will use

$$\hbar = 1.054\,571\,8 \times 10^{-34} \text{ J} \cdot \text{s}, \quad h = 6.626\,070\,15 \times 10^{-34} \text{ J} \cdot \text{s}, \quad m_e = 9.109\,383\,56 \times 10^{-31} \text{ kg}.$$

The electron density is given: $N = 5 \times 10^{18}$ cm$^{-3}$ $= 5 \times 10^{24}$ m$^{-3}$.

**(a).** For an infinite well with walls at $x = 0$ and $x = L$, the $m$th stationary state has $m$ half- wavelengths that fit inside the well:

$$\frac{\lambda_m}{2} = \frac{L}{m} \quad \Longrightarrow \quad \lambda_m = \frac{2L}{m}.$$

So, as a function of $m$ and $L$,

$$\boxed{\lambda_m = \frac{2L}{m}}.$$

For $L = 2$ nm this gives $\lambda_m = \dfrac{4 \text{ nm}}{m}$ (e.g. $m = 1 \Rightarrow 4$ nm, $m = 2 \Rightarrow 2$ nm, $m = 3 \Rightarrow 1.333$ nm, ...).

**(b).** The wave number is $k = 2\pi/\lambda$, so

$$k_m = \frac{2\pi}{\lambda_m} = \frac{2\pi}{2L/m} = \frac{m\pi}{L}.$$

The normalized eigenfunction is

$$\boxed{\psi_m(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{m\pi x}{L}\right)}, \qquad 0 < x < L.$$

**(c).** The energy of the $m$th level is

$$E_m = \frac{\hbar^2 k_m^2}{2m_e} = \frac{\hbar^2}{2m_e}\left(\frac{m\pi}{L}\right)^2 = \frac{\hbar^2 \pi^2}{2m_e L^2} m^2.$$

Plugging $L = 2 \times 10^{-9}$ m and the constants yields:

$$E_1 \approx 0.0940 \text{ eV}, \quad E_2 \approx 0.3760 \text{ eV}, \quad E_3 \approx 0.8461 \text{ eV}, \quad E_4 \approx 1.5041 \text{ eV}, \quad E_5 \approx 2.3502 \text{ eV}.$$

So the general result is

$$\boxed{E_m = \frac{\hbar^2 \pi^2}{2m_e L^2} m^2.}$$

```
h = 6.62607015e-34;
hbar = 1.054571817e-34;
me = 9.10938356e-31;
L = 2e-9;
eV = 1.602176634e-19;
m = 1:5;
Em = (h^2 .* m.^2) ./ (8*me*L^2) / eV;   % in eV
disp(Em)
```

**(d) Permittivity vs. light frequency.** Only transitions from *occupied* to *empty* levels contribute. Since $m = 1, 2, 3$ are filled and $m \geq 4$ is empty, look at $3 \to 4$, $2 \to 4$, $1 \to 4$, $3 \to 5$, etc. Transition energies:

$$\Delta E_{3\to4} = E_4 - E_3 = 1.5041 - 0.8461 \approx 0.6580 \text{ eV}.$$

The corresponding frequency is

$$f_{34} = \frac{\Delta E_{34}}{h} \approx \frac{0.6580 \times 1.602 \times 10^{-19}}{6.626 \times 10^{-34}} \approx 1.59 \times 10^{14} \text{ Hz},$$

which lies in the specified range. All other allowed transitions from filled levels ($1 \to 4$, $2 \to 4$, $3 \to 5$, ...) end up at higher frequencies ($> 2 \times 10^{14}$ Hz). Therefore, **over the given frequency range the only relevant transition is $3 \to 4$.**

$$\omega_{34} = 2\pi f_{34} \approx 2\pi \times 1.59 \times 10^{14} \text{ rad/s}.$$

So that

$$x_{ni} = \int_0^L x\,\psi_n(x)\,\psi_i(x)\,dx.$$

For infinite wells, a standard integral gives

$$\langle n|x|m\rangle = \frac{2L}{\pi^2}\frac{nm}{(n^2 - m^2)^2}\left[1 - (-1)^{n+m}\right].$$

Nonzero only when $n + m$ is odd. For $n = 4$, $m = 3$ we get

$$\langle 4|x|3\rangle = \frac{2L}{\pi^2}\frac{4 \cdot 3}{(16 - 9)^2}\left(1 - (-1)^7\right) = \frac{2L}{\pi^2}\frac{12}{7^2} \cdot 2 = \frac{48L}{49\pi^2}.$$

At $L = 2$ nm,

$$|\langle 4|x|3\rangle| = \frac{48(2 \times 10^{-9})}{49\pi^2} \approx 3.97 \times 10^{-10} \text{ m} = 0.397 \text{ nm}.$$

Homogenous broadening (half-width) is $\Gamma = 1$ meV $= 10^{-3}$ eV. In joules this is $\Gamma_J = 10^{-3} \times 1.602 \times 10^{-19} \approx 1.602 \times 10^{-22}$ J. The corresponding damping rate is

$$\gamma = \frac{\Gamma_J}{\hbar} \approx 1.52 \times 10^{12} \text{ s}^{-1}.$$

For a single transition $m \to n$ in the dipole approximation,

$$\chi(\omega) = \frac{Ne^2|\langle n|x|m\rangle|^2}{\varepsilon_0\hbar}\left(\frac{1}{\omega_{nm} - \omega - i\gamma} - \frac{1}{\omega_{nm} + \omega + i\gamma}\right),$$

and the permittivity is $\varepsilon(\omega) = \varepsilon_0\left[1 + \chi(\omega)\right]$ (I'm taking background to be 1).

Separating real and imaginary parts (still for one transition):

$$\boxed{\begin{aligned} \mathrm{Re}\{\varepsilon(\omega)\} &= \varepsilon_0\left[1 + \frac{Ne^2|\langle n|x|m\rangle|^2}{\varepsilon_0\hbar}\left(\frac{\omega_{nm} - \omega}{(\omega_{nm} - \omega)^2 + \gamma^2} - \frac{\omega_{nm} + \omega}{(\omega_{nm} + \omega)^2 + \gamma^2}\right)\right], \\ \mathrm{Im}\{\varepsilon(\omega)\} &= \varepsilon_0\frac{Ne^2|\langle n|x|m\rangle|^2}{\varepsilon_0\hbar}\left(\frac{\gamma}{(\omega_{nm} - \omega)^2 + \gamma^2} - \frac{\gamma}{(\omega_{nm} + \omega)^2 + \gamma^2}\right). \end{aligned}}$$

In my script, I just plug in $(n, m) = (4, 3)$.

```
eps0 = 8.8541878128e-12;
e = 1.602176634e-19;
h = 6.62607015e-34;
hbar = 1.054571817e-34;
me = 9.10938356e-31;
L = 2e-9;
N = 5e24;                 % m^-3
x43 = 96*L/(49*pi^2);    % same as 48L/(49pi^2), numerically ~3.97e-10 m
```

```

E3 = 0.8460678790*e;
E4 = 1.5041206738*e;
dE = E4 - E3;
omega0 = dE / hbar;      % rad/s

Gamma_eV = 1e-3;
gamma = (Gamma_eV*e)/hbar;

f = linspace(1e14, 2e14, 1000);
omega = 2*pi*f;

pref = N*e^2*x43^2/(eps0*hbar);
chi = pref.*( 1./(omega0 - omega - 1i*gamma) ...
            - 1./(omega0 + omega + 1i*gamma) );
eps_complex = eps0*(1 + chi);

eps_real = real(eps_complex);
eps_imag = imag(eps_complex);
```

**(e) Maximum optical absorption coefficient.**

$$\alpha(\omega) = \frac{\omega}{c}\,\mathrm{Im}\{n(\omega)\}, \qquad n(\omega) = \sqrt{\frac{\varepsilon(\omega)}{\varepsilon_0}}.$$

Evaluating this numerically gives a peak at the transition frequency $f \approx 1.59 \times 10^{14}$ Hz, with

$$\alpha_{\max} \approx 9.7 \times 10^6 \text{ m}^{-1} = 9.7 \times 10^4 \text{ cm}^{-1}.$$

So,

$$\boxed{\alpha_{\max} \approx 1 \times 10^5 \text{ cm}^{-1} \text{ at } f \approx 1.59 \times 10^{14} \text{ Hz.}}$$

```
c = 299792458;
n_complex = sqrt(eps_complex/eps0);
alpha = omega./c .* imag(n_complex);    % 1/m
[alpha_max, idx] = max(alpha);
f_at_max = f(idx);
fprintf('alpha_max = %.3e 1/m at f = %.3e Hz\n', alpha_max, f_at_max);
```

**(f) Matching to a classical bound-electron model.** A classical oscillator for number density $N_a$ has

$$\chi_{\mathrm{cl}}(\omega) = \frac{N_a e^2}{\varepsilon_0 m_e} \frac{1}{\omega_0^2 - \omega^2 - i\gamma'\omega},$$

with resonance $\omega_0$, damping $\gamma'$ and spring constant $k = m_e\omega_0^2$.

Near resonance ($\omega \approx \omega_0$), this becomes

$$\chi_{\mathrm{cl}}(\omega) \approx \frac{N_a e^2}{2\varepsilon_0 m_e \omega_0} \frac{1}{\omega_0 - \omega - i\gamma'/2}.$$

And our previous quantum mechanical expression near resonance ($3 \to 4$) is

$$\chi_{\mathrm{qm}}(\omega) \approx \frac{N e^2 |\langle 4|x|3\rangle|^2}{\varepsilon_0 \hbar} \frac{1}{\omega_{34} - \omega - i\gamma}.$$

Matching the coefficients and the linewidths gives

$$\frac{N_a e^2}{2\varepsilon_0 m_e \omega_0} = \frac{N e^2 |\langle 4|x|3\rangle|^2}{\varepsilon_0 \hbar} \quad \Longrightarrow \quad \boxed{N_a = N \frac{2 m_e \omega_0 |\langle 4|x|3\rangle|^2}{\hbar}},$$

and to match the linewidths

$$\frac{\gamma'}{2} = \gamma \quad \Longrightarrow \quad \boxed{\gamma' = 2\gamma}.$$

Using the numbers above:

$$\omega_0 = \omega_{34} \approx 2\pi \times 1.59 \times 10^{14} \text{ rad/s},$$
$$|\langle 4|x|3\rangle| \approx 3.97 \times 10^{-10} \text{ m},$$
$$N = 5 \times 10^{24} \text{ m}^{-3}, \quad m_e = 9.11 \times 10^{-31} \text{ kg}.$$

This gives

$$N_a \approx 1.36 \times 10^{25} \text{ m}^{-3},$$

so of the same order (but a bit larger than) the actual electron density in the well.

The resonance frequency in Hz is

$$\boxed{f_0 = \frac{\omega_0}{2\pi} \approx 1.59 \times 10^{14} \text{ Hz},}$$

the damping is

$$\boxed{\gamma' \approx 3.0 \times 10^{12} \text{ s}^{-1},}$$

and the corresponding spring constant in the classical picture is

$$\boxed{k = m_e \omega_0^2 \approx 0.91 \text{ N/m}.}$$

So the best fit parameters to the classical model to emulate the quantum $3 \to 4$ transition are roughly

$$\boxed{N_a \simeq 1.4 \times 10^{25} \text{ m}^{-3},\ f_0 \simeq 1.6 \times 10^{14} \text{ Hz},\ \gamma' \simeq 3 \times 10^{12} \text{ s}^{-1},\ k \simeq 0.9 \text{ N/m}.}$$