* Perturbation Theory handout – complete step 4

Final Pert Theory note:

$$U_{kk'} = \int \psi_k^{0*} U(\vec{r}) \psi_{k'}^{0} \, dV$$

$$= \frac{1}{V} \int U(\vec{r}) \, e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} \, dV \quad \text{(as discussed)}$$

Also as discussed, $\vec{k}' - \vec{k} = \vec{G}$ to give a nonzero integral

so $U_{kk'}$ really $= \frac{1}{V} \int U(\vec{r}) \, e^{i\vec{G}\cdot\vec{r}} \, dV$

compare to $\frac{2}{L} \int f(x) \cos \frac{2\pi n x}{L} \, dx$

or $\frac{1}{L} \int f(x) \, e^{i 2\pi n x / L} \, dx$

Fourier coefficient of $n^{th}$ term

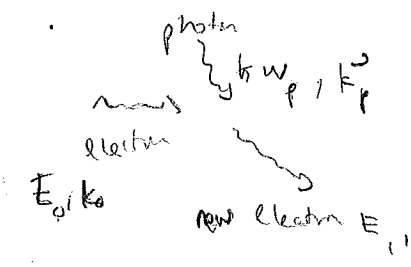
$U_{kk'}$ = Fourier coeff associated w/ G!

$= U_{\vec{G}}$ in Kittel's notation from Central Equation. ☺

Things fit together!

Another fit: both Central Eqn approach + Pert Theory approach predicted that only states related to $\vec{k}$ via RLV will couple together.

Photon Absorption (Not really in Ch 7, but seems to fit here)




cons. energy: $E_0 + \hbar\omega_p = E_1$

cons. momentum: $\vec{k}_0 + \vec{k}_p = \vec{k}_1 \pm \vec{G}_{RLV}$

used reduced zone scheme

$\vec{k}_0 + \vec{k}_p = \vec{k}_1$

↳ can be in different band

Consider magnitudes of numbers

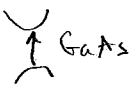
visible light $\lambda \simeq 500\,nm \rightarrow k = \frac{2\pi}{\lambda} = \frac{2\pi}{(500)\cdot 10^{-9}} \simeq \underline{10^7\ m^{-1}}$

Also: $E_{photon} \simeq 1\text{-}3\,eV$

size of BZ: $\frac{2\pi}{a} \simeq \frac{2\pi}{5\cdot 10^{-10}\,m} \simeq \underline{10^{10}\ m^{-1}}$

Conclusion: optical transitions look vertical

only go over $\simeq .1\%$ of BZ




Indirect transitions:

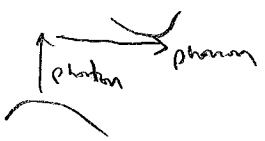
recall phonon energy scales: $f \simeq 5\cdot 10^{12}\,Hz$ (fig 8, pg 96)

$E = hf \Rightarrow \underline{E = .021\,eV}$

and yet phonon k values include whole BZ

⇒ phonon transitions look horizontal

combo transitions called "indirect"




optical absorption at $E_g$ less likely

because need to absorb a phonon as well

(Si can't emit light easily also, for same reason)

but GaAs = great!