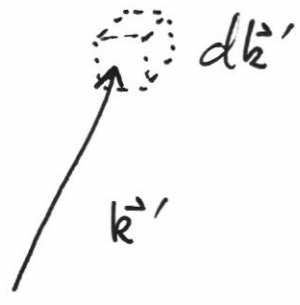


Last time



Initial  $e^-$  wave fn



Final  $e^-$  wave fn

$$\text{Probability} = \frac{2\pi}{\hbar} \underbrace{\left| \langle \vec{k} | H' | \vec{k}' \rangle \right|^2}_{\substack{\text{matrix element} \\ \text{for transition}}} \text{DOS}(\vec{k}) d\vec{k}' dt$$

~~last time~~

$$\langle \vec{k} | H' | \vec{k}' \rangle = \int u_{\vec{k}}^*(\vec{r}) \vec{u}_{\vec{k}'_{ph}} \cdot \frac{dV}{d\vec{r}} u_{\vec{k}'}(\vec{r}) d\vec{r}$$

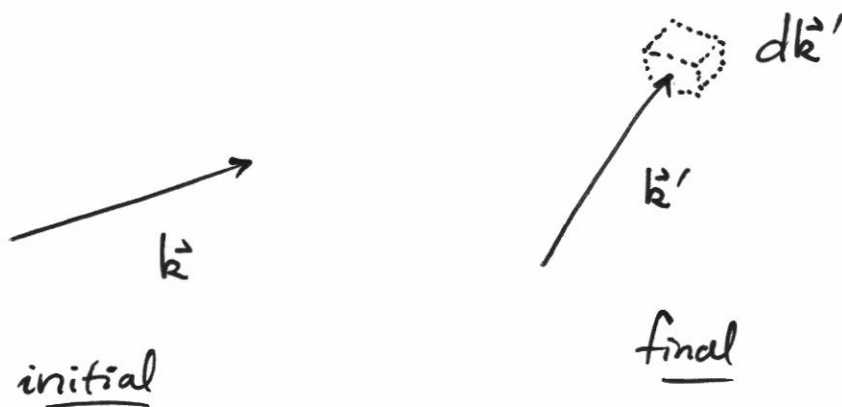
if energy & momentum are conserved

$$\left| \langle \vec{k} | H' | \vec{k}' \rangle \right|^2 = n_{\text{phonon}} \underbrace{\left| g_{\vec{k}\vec{k}'} \right|^2}_{\substack{\text{electron phonon coupling} \\ \text{constant for a given} \\ \vec{k} \ \& \ \vec{k}' \dots \text{ a material} \\ \text{property.}}}$$

Since  $E \propto n_{\text{phonon}} \propto (\text{displacement})^2$   
Depends on T.

(2) ~~(1)~~

Put the matrix element back into Fermi's Golden Rule:



$$\text{Prob} = \frac{2\pi}{\hbar} \left| \langle \vec{k} | H' | \vec{k}' \rangle \right|^2 \text{DOS}(\vec{k}') d\vec{k}' dt$$

$$= \frac{2\pi}{\hbar} \frac{1}{e^{\hbar\omega_{ph}/k_B T} - 1} \left| g_{\vec{k}\vec{k}'} \right|^2 \text{DOS}(\vec{k}') d\vec{k}' dt$$

You can see why the single relaxation time approximation often saves time!

As long as energy and momentum are conserved.

Some physical insights from this formula:

If  $k_B T \gg \hbar\omega_{ph}$  (for all  $\omega_{ph}$ )

$$\text{Prob} \propto \frac{1}{e^{\hbar\omega_{ph}/k_B T} - 1} \approx \frac{1}{1 + \frac{\hbar\omega_{ph}}{k_B T} - 1} = \frac{k_B T}{\hbar\omega_{ph}}$$

For all phonon modes

(3) (11)

Resistance  $\propto T$ .

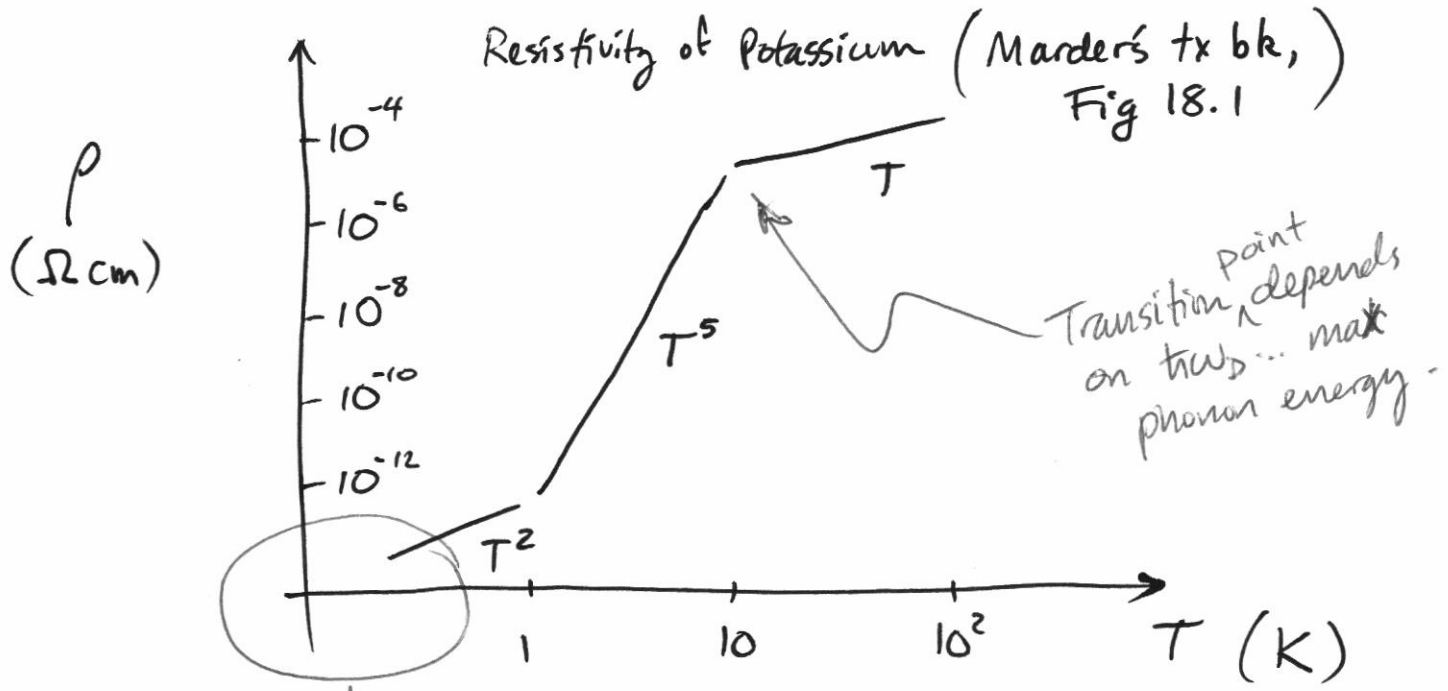
If  $k_B T < \hbar \omega_{ph}$

$$\frac{1}{e^{\hbar \omega_{ph} / k_B T} - 1} \rightarrow 0$$

for some  $\omega_{ph}$ .

~~Some~~ Scattering events are suppressed for large  $\omega_{ph}$  but not small  $\omega_{ph}$ .

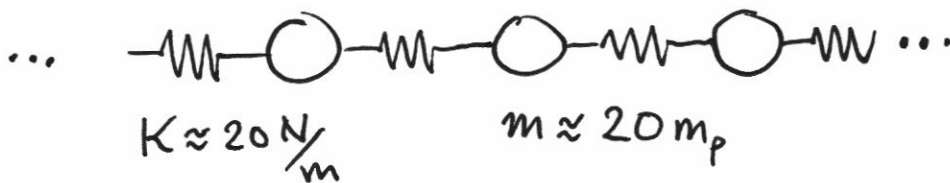
Resistance is not proportional to  $T$ .



④ ~~④~~

The max value of  $\hbar\omega_{ph}$  is a very important energy in  $e^-$  transport theory.

EXERCISE: Estimate  $[\hbar\omega_{ph}]_{\max}$  if



(show the highest freq normal mode on the ~~plot~~ animation/simulation).

5

The temperature dependence of resistivity is our first concrete example where the QM treatment of  $e^-$  transport takes us beyond the Drude model.

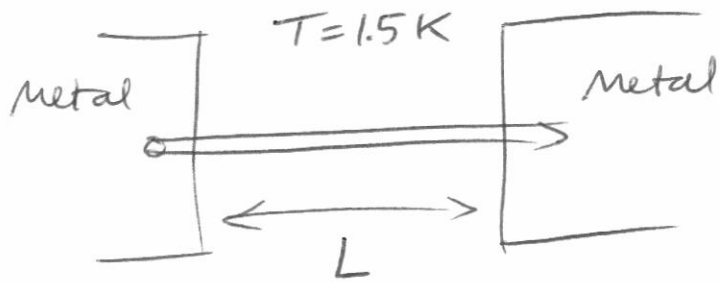
Rest of ~~course~~ PH671: Many more examples where the QM description predicts/explains new phenomena.

**CASE 1** | Cool down a perfect lattice to  $T=0$   
No scattering.

Assume a normal metal (not superconducting)  
Is there any remaining "resistance"? ?

⑥

This expt has been done with CNTs



Liang et al.  
Nature 411 665  
(2001)

$$I = \frac{4e^2}{h} V$$
$$= \frac{V}{6.5 \text{ k}\Omega}$$

Independent of  $L$ .

There is nothing to cause scattering.

Apply QM description of  $e^-$  transport to this system.