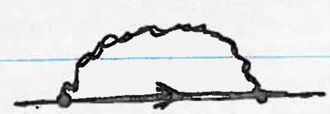
Polaron in the weak coupling limit

Consider a semiconductor. Electrons in a conduction band represent a diluted gas. When concentration is small, electron-electron interactions can be neglected.

At the same time, ~~a single~~ an injected electron, while moving in ~~the~~ a cristalized lattice, it polarises surrounding medium and leads to a deformation of the lattice. These deformations are nothing but phonons. Such an electron, which is surrounded by a cloud of phonons, is called polaron.

Polaronic dispersion is: $\varepsilon(\vec{p}) = \varepsilon_0 + \frac{p^2}{2m^*}$

~~ε_0~~ m^* - effective mass, which we will calculate.
To be more specific, we let us calculate the ~~lowest order~~ electron self-energy in the lowest order in e-ph interactions. It is given by this diagram

$\Sigma =$  where $G(\varepsilon, \vec{p}) = \frac{1}{\varepsilon - p^2/2m + i\delta}$,

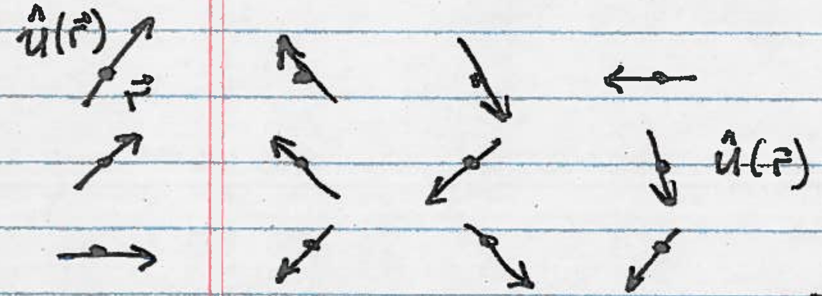
$\delta > 0 \Leftrightarrow$ electron tunnels into the semiconductor from outside, ~~and there~~ where was in the conduction zone there were no electrons before.

We calculate $\Sigma(\varepsilon, \vec{p})$ in the vicinity of the mass-shell defined by a condition $\varepsilon = p^2/2m$, and at $|p| \ll mc$.

Electron-phonon interactions

Let $\hat{u}(\vec{r},t)$ be the operator associated with

displacements of atoms on a lattice.



$\hat{u}(\vec{r})$ forms dipol moment and induces $\boxed{\text{polarization}}$ $\boxed{\text{density}}$

$$\vec{P}(\vec{r}) = e \cdot \frac{N}{V} \cdot \hat{u}(\vec{r})$$

N - total # of ~~atoms~~ (ions)
V - total volume.

Generally, ~~that~~ the electric displacement field (induced field) is given by

$$\vec{D} = \underset{\text{(vacuum) dielectric constant}}{\varepsilon_0} \cdot \vec{E} + 4\pi \vec{P}(\vec{r}) = \varepsilon \cdot \vec{E}$$

From Maxwell equations we have $(\vec{E}=0)$

$$\operatorname{div} \vec{D} = 4\pi \rho \implies \boxed{\operatorname{div} \vec{P}(\vec{r}) = \rho_c} \sim \operatorname{div} \hat{u}(\vec{r})$$

→ where ρ_c is $\boxed{\text{the electric charge density}}$ induced by the displacement field, $\hat{u}(\vec{r})$.

Deformation potential $\quad V(\vec{r}) = g \cdot \hat{\varphi}(\vec{r}) = c\sqrt{\rho}\, \operatorname{div} \hat{u}(\vec{r})$
$\sim \rho_c$.

Interaction Hamiltonian is ~~a product of dens~~ given by a product of densities:

electron density $\qquad\qquad\qquad$ electric charge density.

$$H_{int} \sim g \int n(\vec{r})\, K(\vec{r}-\vec{r}')\, \mathrm{div}\, \vec{P}(\vec{r}')\, d^3\vec{r}\, d^3\vec{r}'$$

where K is an interaction function.

$$K(\vec{r}-\vec{r}') \simeq \begin{cases} \dfrac{1}{|\vec{r}-\vec{r}'|}, & |\vec{r}-\vec{r}'| \lesssim a \\ 0, & |\vec{r}-\vec{r}'| \gg a \end{cases}$$

Approximation: $\underline{K(\vec{r}-\vec{r}') = \#\cdot\delta(\vec{r}-\vec{r}')} \Rightarrow$

$$\Rightarrow \quad \hat{H}_{int} = g \int \hat{\psi}^+(\vec{r})\, \psi(\vec{r})\, \hat{\varphi}(\vec{r})\, d^3\vec{r}.$$

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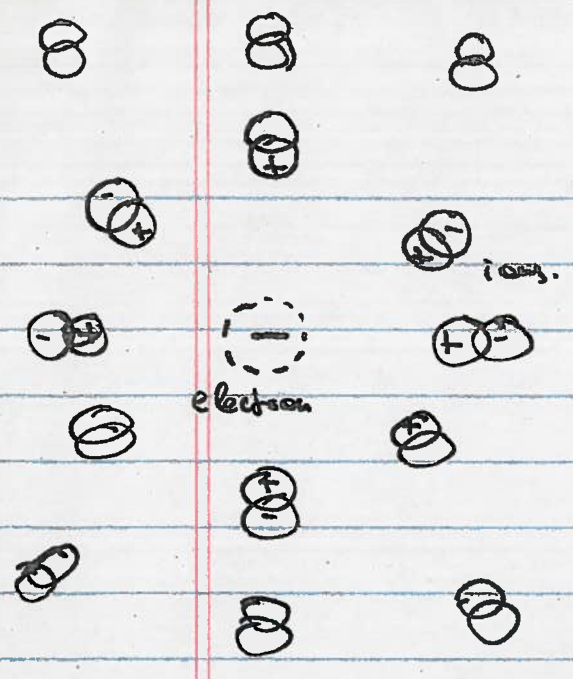
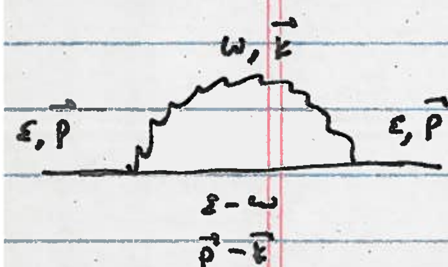
5. Electron-phonon interaction

1. Fröhlich Hamiltonian.
2. Polaron in a weak coupling limit.
3. Cherenkov radiation of sound.



Polaron: single electron

polarizes surrounding medium and leads to a deformation of the lattice. These deformation are phonons. As a result the electronic effective mass changes.



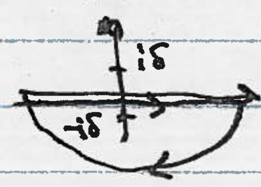
$$= \sum (\varepsilon, \vec{p}) = i g^2 \int G_0(\varepsilon - \omega, \vec{p} - \vec{k}) D_0(\omega, \vec{k}) \frac{d^3k}{(2\pi)^3} \frac{d\omega}{2\pi}$$

where $G_0(\varepsilon, \vec{p}) = \dfrac{1}{\varepsilon - p^2/2m + i\delta}$ - electron Green's function

$D_0(\omega, \vec{k}) = \dfrac{c^2 k^2}{\omega^2 - c^2 k^2 + i\delta}$ - phonon Green's function.

Let us adopt the following sequence of integration:

1. over ω. $\int_{-\infty}^{\infty} d\omega \rightarrow$ choose



$$D_0(\omega, \vec{k}) = \frac{\omega_0(k)}{2} \left[\frac{1}{\omega - \omega_0(k) + i\delta} - \frac{1}{\omega + \omega_0(k) - i\delta} \right]$$

Let me first state the result, and then do ~~the~~ calculations. The result reads:

$$\Sigma(\varepsilon, \vec{p}) = \varepsilon_0 - \alpha_1 \left(\varepsilon - \frac{p^2}{2m}\right) - \alpha_2 \frac{p^2}{2m}$$

From here we can conclude that

1) α_2 - determines the mass renormalization: $\frac{m_*}{m} = f(\alpha_2)$

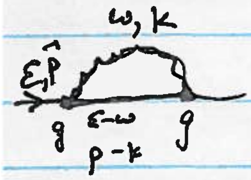
Qualitatively this can be understood from the following reasoning....

2) α_1 - determines renormalization of fermionic residue, Z, which is not 1 anymore.

__proof:__

$$\cancel{G = \frac{1}{G_0^{-1} - \Sigma} = \frac{1}{\left[\varepsilon - \frac{p^2}{2m} + i\delta\right] - \varepsilon_0 - \alpha_1\left[\varepsilon - \frac{p^2}{2m}\right] - \alpha_2 \frac{p^2}{2m}} =}$$

calculation of the self-energy diagram:



$$= \Sigma(\varepsilon, \vec{p}) = i g^2 \int G_0(\varepsilon - \omega, \vec{p} - \vec{k})\, D_0(\omega, \vec{k}) \frac{d^3k}{(2\pi)^3} \frac{d\omega}{2\pi},$$

where $$G_0(\varepsilon, \vec{p}) = \frac{1}{\varepsilon - p^2/2m + i\delta},$$

$$D_0(\omega, k) = \frac{c^2k^2}{\omega^2 - c^2k^2 + i\delta}.$$

Let us perform integration over ω closing the contour in the lowest half-plane:

$$\int_{-\infty}^{+\infty} \frac{1}{\tilde{\mathcal{E}} - \omega + i0} \, \frac{c^2 k^2}{\omega^2 - c^2 k^2 + i0} \, \frac{d\omega}{2\pi} = \frac{i}{2} \, \frac{ck}{ck - \tilde{\mathcal{E}} - i0} . \to \underline{\text{prove.}}$$

where $\tilde{\mathcal{E}} = \mathcal{E} - \frac{(p-k)^2}{2m}$, $k = |\vec{k}|$. Therefore we got

$$\Sigma(\varepsilon, \vec{p}) = \frac{g^2}{2} \int \frac{ck}{\varepsilon - ck - \frac{(p-k)^2}{2m} + i0} \, \frac{d^3k}{(2\pi)^3}$$

As the next step we make use of the following trick:
Integration over d^3k can be performed as follows.

Introduce $k = |\vec{k}|$, $q = |\vec{p} - \vec{k}|$, $x = \cos \widehat{\vec{k}\vec{p}} \Rightarrow$

$$\Rightarrow d^3k = 2\pi k^2 \, dk \, dx \quad , \text{while } q^2 = |\vec{p} - \vec{k}|^2 = $$
$$= p^2 + k^2 - 2pk\,x \Rightarrow$$

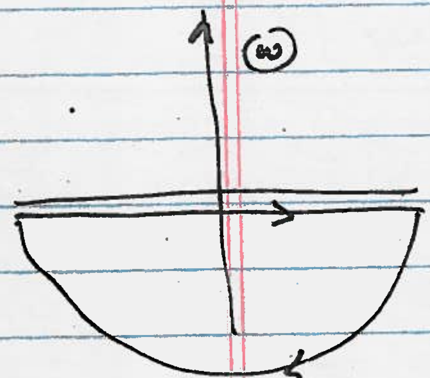
$$\Rightarrow q\,dq = -pk\,dx .$$

We obtain that

$$\int f\left(|\vec{k}|, |\vec{p} - \vec{k}|\right) \frac{d^3k}{(2\pi)^3} \equiv \frac{1}{(2\pi)^2 \cdot p} \int k\,dk \int_{|p-k|}^{|p+k|} f(k, q)\, q\, dq$$

$$\Sigma(\varepsilon, \vec{p}) = ig^2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} \cdot \underbrace{\frac{1}{\varepsilon - \omega - (\vec{p}-\vec{k})^2/2m + i\delta}}_{\text{pole in the upper half-plane.}} \times$$

$$\times \frac{\omega_0(k)}{2} \left[\underbrace{\frac{1}{\omega - \omega_0(k) + i\delta}}_{\text{pole in the lower h.p.}} - \underbrace{\frac{1}{\omega + \omega_0(k) - i\delta}}_{\text{upper.}} \right] =$$



$$= -2i\pi \cdot ig^2 \cdot \frac{1}{2\pi} \cdot \frac{1}{2} \frac{\omega_0(k)}{\varepsilon - \omega_0(k) - \frac{(p-k)^2}{2m} + i\delta}$$

$$= \frac{g^2}{2} \cdot \int \frac{\omega_0(k)}{\varepsilon - \omega_0(k) - \frac{(\vec{p}-\vec{k})^2}{2m} + i\delta} \frac{d^3k}{(2\pi)^3}.$$

Analysis of the expression.

Let us analyze whether there is imaginary part and wh[en] imaginary part is zero.

$x_{min} = (p-k)^2$, => if argument of δ-function is > 0 always

then $\operatorname{Im}\Sigma = 0$.

We have $(p-k)^2 - 2m\left[\varepsilon - ck\right] > 0.$

$$\cancel{p^2} + k^2 - 2pk - 2m\cancel{\frac{p^2}{2m}} + 2mck > 0$$

$$k + 2(mc - p) > 0$$

Lower: small. and ≥ 0 if $\boxed{(mc-p) > 0 \Rightarrow \operatorname{Im}\Sigma = 0}$

Which yields

$$\Sigma = \frac{g^2}{2(2\pi)^2 p}\int_0^{k_D} k\,dk \int_{|p-k|}^{p+k} \frac{ckq\,dq}{\varepsilon - q^2/2m - ck + i0}\,, \qquad \boxed{\frac{1}{x+i0} = \frac{1}{x} - i\pi\delta(x)}$$

Now we integrate over $x = q^2$:

IMPORTANT EXPRESSION

$$\Sigma = \frac{g^2 mc}{8\pi^2 p}\int_0^{k_D} \ln\left|\frac{\varepsilon - (p-k)^2/2m - ck}{\varepsilon - (p+k)^2/2m - ck}\right| k^2 dk -$$

$$- i\,\frac{g^2 mc}{8\pi p}\int_0^{k_D} k^2 dk \int_{(p-k)^2}^{(p+k)^2} \delta\big(x - 2m(\varepsilon - ck)\big)\,dx$$

Analysis.

When $p < mc$, $\Rightarrow$ Σ is real $\Rightarrow$ polaron is stable!

Effects coming from $p > mc$ will be discussed on Wednesday.

We are interested in Σ near the mass-shell $\varepsilon = p^2/2m$

and when p is small. $p \ll mc$, $\Delta = \left(\varepsilon - \frac{p^2}{2m}\right) \ll ck$, $v = p/m$

Expanding in $\frac{\Delta}{ck}$ and $\frac{v}{c}$ we obtain

$$(p-k)^2 < 2m\left(\frac{p^2}{2m} - ck\right) < (p+k)^2 \qquad k, p > 0$$

$\mathrm{Im}\,\Sigma$ is finite

is equivalent to $\boxed{0 < k < 2(p - mc)}$ $\Rightarrow$ ~~[illegible]~~

$$\Sigma = \frac{g^2 mc}{8\pi^2 p} \int_0^{k_D} \ln \left| \frac{k^2/2m + (c-v)k - \Delta}{k^2/2m + (c+v)k - \Delta} \right| k^2 dk =$$

$$= \frac{g^2 mc}{8\pi^2 p} \int_0^{k_D} \left(- \frac{2vk}{ck + k^2/2m} - \frac{4\Delta vk}{2(ck + k^2/2m)^2} - \frac{2v^3k^3}{3(ck + k^2/2m)^3} + \ldots \right) \times$$

$$\times k^2 dk$$

These three terms yield

$\Sigma = \varepsilon_0 - \alpha_1 \Delta - \alpha_2 \, p^2/2m$ form of Σ. Moreover, since $\boxed{c \ll k_D/m}$, in denominators we can safely neglect kc with respect to $k^2/2m$. This yields:

$$\varepsilon_0 = - \frac{g^2 c}{4\pi^2} \int_0^{k_D} \frac{k^3 dk}{ck + k^2/2m} = - \frac{g^2 mc k_D^2}{4\pi^3} .$$

Within log accuracy we have.

$$\alpha_1 = \frac{g^2 m^2 c}{\pi^2} \int_0^{k_D} \frac{k^3 dk}{(k^2 + 2mck)^2} = \frac{g^2 m^2 c}{\pi^2} \ln \frac{k_D}{mc}$$

$$G_0^{-1} - \Sigma = \omega - \frac{p^2}{2m} - \varepsilon_0 + \alpha_2 \frac{p^2}{2m} \to \omega - \frac{p^2}{2m}(1 - \alpha_2)$$

$$\alpha_2 = \frac{2g^2 m^3 c}{3\pi^2} \cdot \frac{2}{m} \int_0^{k_D} \frac{k^5 dk}{(k^2 + 2mck)^3} = \frac{4g^2 m^2 c}{3\pi^2} \ln \frac{k_D}{mc} = \frac{4}{3} \alpha_1 .$$

Dispersion relation is determined from $G_0^{-1} - \Sigma = 0 \Rightarrow$

$\Rightarrow \dfrac{m_*}{m} = \dfrac{1}{1 - \alpha_2} > 1 \to$ electron dressed rather than undressed.

4. Now let us turn to the next problem:

<u>Cherenkov radiation of sound.</u>

We will show that $\Sigma_1(\varepsilon, \vec{p})$ self-energy has a finite imaginary part when $\boxed{v = p/m > c}$. This is because if electron is faster than sound, it emits phonons.

From $(*)$ we see that integration over x yields a finite value if.

$$(p-k)^2 < 2m\left(\frac{p^2}{2m} - ck\right) < (p+k)^2 \qquad k, p > 0.$$

This condition is equivalent to $\boxed{0 < k < 2(p-mc)}$, and therefore $\mathrm{Im}\,\Sigma$ is finite when $\boxed{v = p/m > c}$.

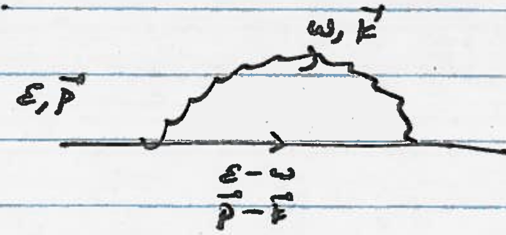
Probability to emit a photon in unit time is given by

$$2\gamma = -2\,\mathrm{Im}\,\Sigma_1 = 2\,\frac{g^2\, mc}{8\pi p}\int_0^{2m(v-c)} k^2\, dk = \frac{2g^2 m^3}{3\pi}\,\frac{c}{v}\cdot(v-c)^3$$

From here we see that electron emits phonons when $\boxed{v > c}$. Probability of emission of a phonon decreases when $v \to c$ and vanishes when $v < c$.

Now let us find the angular distribution of intensity of emitted sound.

We have such a process:



Electron has momentum

$$\vec{q} = \vec{p} - \vec{k} \quad \Rightarrow \quad q^2 = k^2 + p^2 - 2pk \cos\theta .$$

From conservation of energy we have $\dfrac{p^2}{2m} = \dfrac{q^2}{2m} + ck$.

Therefore $\cos\theta = \dfrac{(k + 2mc)}{2p}$ and we can pass from $\boxed{dk \to d\theta}$.

Then the imaginary part of the self-energy reads:

$$\mathrm{Im}\,\Sigma = -\frac{g^2 m c}{8\pi p} \int_0^{2m(v-c)} k^2 dk = \frac{g^2 m c}{4\pi} \int_0^{\theta_{max}} \left[2p\cos\theta - 2mc\right]^2 d|\cos\theta| =$$

$$= \frac{g^2 (mc)^3}{\pi} \int_0^{\theta_{max}} \left(\frac{v}{c}\cos\theta - 1\right)^2 \sin\theta \, d\theta$$

where $\theta_{max} = \arccos(c/v)$ - maximal ~~value of~~ angle under which a phonon can be emitted.

Integrand $f(\theta) = \# \cdot \left(\dfrac{v}{c}\cos\theta - 1\right)^2 \cdot \sin\theta$ defines the angular distribution of intensity of the emitted sound inside a cone with angle θ_{max}.

$\delta(\omega + \omega_0(k))$ in $\operatorname{Im} D_0$ can be neglected as it corresponds to absorption of a phonon. Thus we obtain:

$$\operatorname{Im} \Sigma = -\frac{\pi^2}{2} g^2 \int \omega_0(\vec{k})\, \delta\left(\varepsilon - \omega - \frac{(\vec{p}-\vec{k})^2}{2m}\right) \delta(\omega - \omega_0(\vec{k}))\, \frac{d^3k}{(2\pi)^3} \frac{d\omega}{2\pi}$$

Integration over ω is straightforward and yields

$$\operatorname{Im} \Sigma(\varepsilon, \vec{p}) = -\frac{\pi}{4} g^2 \int \omega_0(k)\, \delta\left(\varepsilon - \omega_0(k) - \frac{(\vec{p}-\vec{k})^2}{2m}\right) \frac{d^3k}{(2\pi)^3}$$

Taking $\operatorname{Im}\Sigma$ on a mass shell we obtain

$$\operatorname{Im} \Sigma\left(\varepsilon = \frac{p^2}{2m}, \vec{p}\right) = -\frac{\pi}{4} g^2 c \int \delta\left(\frac{k}{2m} + c - \frac{p}{m}\cos\theta\right) \frac{k^2\, dk}{(2\pi)^2} \sin\theta\, d\theta$$

We integrate over k with the help of the δ-function which yields the same expression we had before.

This is the same Cherenkov effect but for electrons and phonons.

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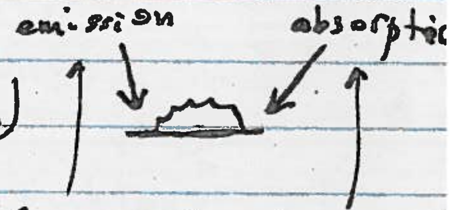
4. b) <u>Second solution:</u>

Physical meaning of $\text{Im}\,\Sigma$ is inverse time ~~[illegible]~~ ~~[illegible]~~ decay into an electron and phonon. Resultant particles, electron and phonon are real particles, which means that their energies and momenta are connected through dispersion relations. Therefore, to calculate $\text{Im}\,\Sigma$ it is sufficient to extract the contribution coming from mass-shell of intermediate particles:



$$G_0(\varepsilon,\vec{p}) \to \text{Im}\, G_0(\varepsilon,\vec{p}) = -i\pi\,\delta(\varepsilon - p^2/2m)$$

$$D_0(\omega,\vec{k}) \to \text{Im}\, D_0(\omega,\vec{k}) = -\,i\,\frac{\pi}{2}\,\omega_0(k)\left[\delta(\omega-\omega_0(k)) + \delta(\omega+\omega_0(k))\right]$$

In other words ~~pa~~ intermediate particles are not virtual. They are real and therefore

$$\text{Im}\,\Sigma = g^2 \int \text{Im}\, G_0(\varepsilon-\omega,\vec{p}-\vec{k})\, \text{Im}\, D_0(\omega,\vec{k})\, \frac{d^3k}{(2\pi)^3}\, \frac{d\omega}{2\pi}.$$

But formally speaking this is an exact mathematical identity.