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Examen de physique statistique hors équilibre
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$\boxed{\text{Peierls instability in 1D metals}}$

A. Compressibility of the 1D electronic gas

free electrons in 1D. $\begin{cases} \epsilon_k = \frac{k^2}{2m}\,, & k \in \mathbb{R} \\ \psi_k = \frac{1}{\sqrt{L}}\, e^{ikx} \end{cases}$

1) $\hat{n}(x)$: 1e⁻ density operator

$\hat{n}_q = e^{-iq\hat{x}}$ $\qquad \langle \psi_k | \hat{n}_q | \psi_{k'} \rangle = \int \frac{dx}{L}\, e^{-ikx - iqx + ik'x} = \delta_{k', k+q}$

2) $\hat{H}_{pert}(t) = \frac{1}{L} \sum_q V_q(t)\, \hat{n}_{-q}$

$\langle \hat{n}_q(t) \rangle = n \cdot L\, \delta_{q,0} + \int dt'\, \tilde{\chi}_q(t-t')\, V_q(t') + \dots$

a) $\tilde{\chi}_q(t) = -i\, \theta_H(t)\, \langle [\hat{n}_q(t), \frac{n_{-q}}{L}] \rangle$

b) $\tilde{\chi}(q,\omega) = \frac{-i}{L} \int_0^\infty dt\, e^{i\omega t} \underbrace{\langle [\hat{n}_q(t), n_{-q}] \rangle}$

$\sum_{k,k'} (f_k - f_{k'})\, (\hat{n}_q)_{kk'}\, e^{i(\epsilon_k - \epsilon_{k'})t}\, (\hat{n}_{-q})_{k'k}$

$|\underbrace{(\hat{n}_q)_{kk'}}_{\delta_{k',k+q}}|^2$

$= \sum_k (f_k - f_{k+q})\, e^{i(\epsilon_k - \epsilon_{k+q})t}$

$= -\frac{i}{L} \sum_k \frac{f_k - f_{k+q}}{0^+ - i(\omega + \epsilon_k - \epsilon_{k+q})} \Rightarrow \boxed{\tilde{\chi}(q,\omega) = \frac{1}{L} \sum_k \frac{f_k - f_{k+q}}{\omega + \epsilon_k - \epsilon_{k+q} + i0^+}}$

poles have neg. imaginary part (causality)

poles are $\omega_q = \underline{\epsilon_{k+q} - \epsilon_k}$ = energy of particle hole excitation

with $\begin{cases} \epsilon_{k+q} > \epsilon_F \\ \epsilon_k < \epsilon_F \end{cases}$

3) Static compressibility

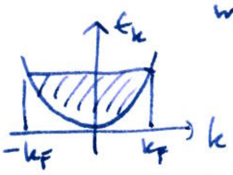
$\frac{f_k}{\epsilon_{k+q} - \epsilon_k} - \frac{f_{-k-q}}{\epsilon_{k+q} - k}$ is symmetrized under $k \to -(k+q)$, hence

a) $\chi_T(q) \equiv \tilde{\chi}(q, 0) = -\frac{1}{L} \sum_k \frac{f_k - f_{k+q}}{\epsilon_{k+q} - \epsilon_k}$ — $i0^+$ is useless because numerator vanishes for $\epsilon_{k+q} - \epsilon_k = 0$

$\sum_k \frac{-f_{k+q}}{\epsilon_{k+q} - \epsilon_k} \underset{k+q \to k}{=} \sum_k \frac{-f_k}{\epsilon_k - \epsilon_{k-q}} \underset{\substack{k \to -k \\ \text{with } \epsilon_k = \epsilon_{-k}}}{=} \sum_k \frac{-f_k}{\epsilon_k - \epsilon_{k+q}} = \sum_k \frac{f_k}{\epsilon_{k+q} - \epsilon_k}$

PP

$\boxed{\chi_T(q) = -\frac{2}{L} \sum_k \frac{f_k}{\epsilon_{k+q} - \epsilon_k}}$ $\qquad T=0$



$\epsilon_{k+q} - \epsilon_k = \frac{(k+q)^2}{2m} - \frac{k^2}{2m} = \frac{q^2}{2m} + \frac{qk}{m}$

b) $\boxed{T=0}$: $\chi_0(q) = -2 \fint_{-k_F}^{k_F} \frac{dk}{2\pi}\, \frac{1}{k + \frac{q}{2}}\, \frac{m}{q} = -\frac{2m}{q\,2\pi} \ln\left| \frac{k_F + q/2}{k_F - q/2} \right|$

Principal part

Rq: if $q = 2k_F$, integral diverges because $\int_{-k_F} \frac{dk}{k + k_F} = \infty$

$$\boxed{\chi_0(q) = -\frac{m}{\pi q}\ln\left|\frac{q+2k_F}{q-2k_F}\right|} \qquad \chi_0(q) < 0 \quad \forall q$$

c) $$\chi_0(q) = -\frac{m}{\pi q}\ln\frac{1+q/2k_F}{1-q/2k_F} \xrightarrow[q\to 0]{} -\frac{m}{\pi q}\left(\frac{q}{2k_F}\right)\times 2 = -\frac{m}{\pi k_F} = -\rho_0$$

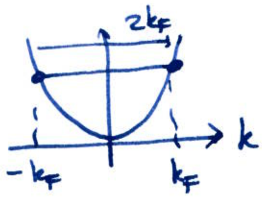
$$\chi_0(q) = -\frac{m}{\pi k_F}\frac{k_F}{q}\ln\frac{1+2k_F/q}{1-2k_F/q} \xrightarrow[q\to\infty]{} -\rho_0\frac{k_F}{q}\left(\frac{2k_F}{q}\times 2\right) = -\rho_0\left(\frac{2k_F}{q}\right)^2$$

$$\chi_0(q) \underset{q\sim 2k_F}{\simeq} -\frac{\rho_0}{2}\ln\frac{4k_F}{|q-2k_F|}$$

4/ Finite T

$$\chi_T(q) = -\frac{1}{\pi}\fint_{-\infty}^{+\infty} dk\,\frac{1}{\epsilon_{k+q}-\epsilon_k}\,\frac{1}{e^{\beta(\epsilon_k-\epsilon_F)}+1}$$

unchanged with T

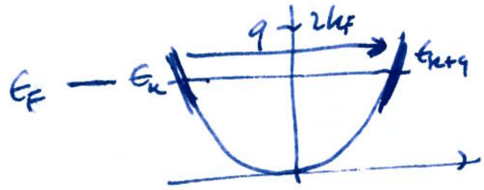


when $q\sim 2k_F \Rightarrow$ integral dominated by $k\sim -k_F$

$\Downarrow$

linearize the spectrum for $k\in[-k_F-k_c, -k_F+k_c]$

cutoff



$$k\sim -k_F \begin{cases} \epsilon_k-\epsilon_F \simeq -v_F(k+k_F) \\ \epsilon_{k+q}-\epsilon_F \simeq v_F(k+q-k_F)\end{cases}$$

$$\chi_T(q) \underset{q\sim 2k_F}{\simeq} -\frac{1}{\pi}\fint_{-k_F-k_c}^{-k_F+k_c} dk\,\frac{1}{v_F(2k+q)}\,\frac{1}{e^{-\beta v_F(k+k_F)}+1}$$

set $u = \beta v_F(k+k_F)$

$$= -\frac{1}{\pi v_F}\fint_{-\beta v_F k_c}^{\beta v_F k_c}\frac{du}{\beta v_F}\,\frac{1}{2\frac{u}{\beta v_F}-2k_F+q}\,\frac{1}{e^{-u}+1}$$

$$\chi_T(q) \underset{q\sim 2k_F}{\simeq} -\frac{\rho_0}{2}\fint_{-\beta\epsilon_c}^{\beta\epsilon_c}\frac{du}{u+\frac{\beta v_F}{2}(q-2k_F)}\,\frac{1}{e^{-u}+1}$$

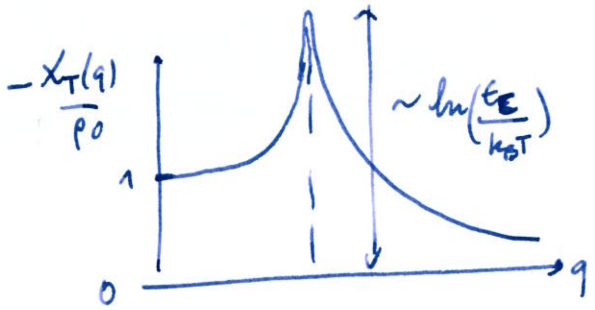
$$\chi_T(2k_F) \simeq -\frac{\rho_0}{2}\fint_{-\beta\epsilon_c}^{\beta\epsilon_c}\underbrace{\frac{du}{u}\,\frac{1}{e^{-u}+1}}_{\text{we symmetrize}} \to \frac{1}{u}\,\frac{1}{2}\Bigg(\underbrace{\frac{1}{e^{-u}+1}-\frac{1}{e^{u}+1}}_{\frac{e^u-e^{-u}}{(e^{-u}+1)(e^u+1)} = \frac{(e^{u/2}-e^{-u/2})(e^{u/2}+e^{-u/2})}{(e^{u/2}+e^{-u/2})^2}}\Bigg)$$

$$= -\frac{\rho_0}{2}\int_0^{\beta\epsilon_c}\frac{du}{u}\,\mathrm{th}\frac{u}{2} = -\frac{\rho_0}{2}\underbrace{\int_0^{\beta\epsilon_c/2}\frac{du}{u}\,\mathrm{th}\,u}_{\simeq\ \ln\left(\frac{4}{\pi}e^{-C}\frac{\beta\epsilon_c}{2}\right)} \qquad = \frac{1}{2u}\,\mathrm{th}\frac{u}{2}$$

$$\Rightarrow \boxed{\chi_T(2k_F) \simeq -\frac{\rho_0}{2}\ln\left(\frac{2e^{-C}}{\pi}\,\frac{\epsilon_c}{k_BT}\right)}$$

is now finite

$\chi_0(2k_F) = -\infty$ is regularised by temperature.



$\chi_T(q) \approx \chi_0(q)$ for q far from $2k_F$

B. Coupling between electrons and phonons.

$$\hat{H}_{pert}(t) = \frac{1}{L}\sum_q V_{-q}(t)\,\hat{n}_q \;\longrightarrow\; \delta E_{elec} = \frac{1}{L}\sum_q V_{-q}\underbrace{\left(\langle \hat{n}_q\rangle_V - \langle \hat{n}_q\rangle\right)}_{\delta\hat{n}_q = \chi_T(q)\,V_q}$$

drop t dependence

$$\boxed{\delta E_{elec} = \frac{1}{L}\sum_q \chi_T(q)\,|V_q|^2 < 0}$$

1) $\Rightarrow$ an extra potential diminishes the energy of the electron gas

2) Phonons. $E_{vib} = \frac{1}{N}\sum_q \frac{1}{2} M\omega_q^2 |\tilde{\xi}_q|^2$

displacement of atoms
$\Downarrow$
induce potential

$$V_q = \sqrt{\lambda a \frac{M}{2}}\,\omega_q\,\tilde{\xi}_q$$

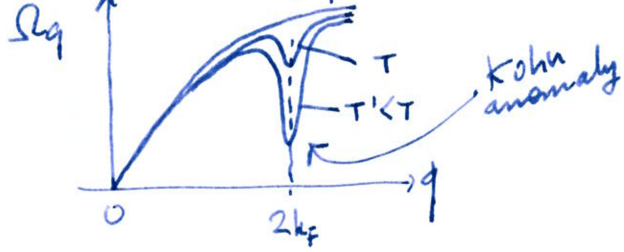
Total energy of the lattice distorsion:

$$\underbrace{\delta E_{elec}}_{e^-\text{ gas}} + \underbrace{E_{vib}}_{\text{elastic energy}} = \frac{1}{L}\sum_q \chi_T(q)\,\lambda a \frac{M}{2}\omega_q^2|\tilde{\xi}_q|^2 + \frac{1}{N}\sum_q \frac{M}{2}\omega_q^2|\tilde{\xi}_q|^2$$

$$= \frac{1}{N}\sum_q \frac{M}{2}\underbrace{\omega_q^2\left(1+\lambda\chi_T(q)\right)}_{\Omega_q^2}|\tilde{\xi}_q|^2$$

Renormalised Phonon spectrum: $\boxed{\Omega_q = \omega_q \times \sqrt{1+\lambda\chi_T(q)}}$

Weak coupling: $\rho_0\lambda \lll 1 \Rightarrow \Omega_q \approx \omega_q$ apart for $q \sim 2k_F$ when $\chi_T(q)$ diverges.



Our approach is valid iff $1+\lambda\chi_T(q) \geq 0 \;\; \forall q$

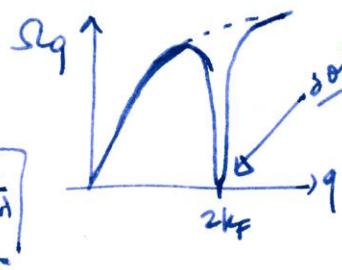
$$\Updownarrow$$

$$\boxed{1+\lambda\chi_T(2k_F) \geq 0}$$

When $1+\lambda\chi_T(2k_F) = 0$

i.e. $1 - \frac{\lambda\rho_0}{2}\ln\frac{2e^{C}}{\pi}\frac{\varepsilon_c}{k_B T} = 0$

i.e. $\boxed{T = T_{Peierls} = \frac{2e^{C}}{\pi}\frac{\varepsilon_c}{k_B}\,e^{-\frac{2}{\rho_0\lambda}}}$



soft mode $\Rightarrow$ modulation at $q = 2k_F$ is costless
$\Downarrow$
Peierls instability

$\rightarrow$ For $T < T_{Peierls}$, the system opens a gap at ε_F in the electronic spectrum $\Rightarrow$ become insulator.