Universités Paris 6, Paris 7 & Paris-Sud, École Normale Supérieure, École Polytechnique
Master 2 CFP – Physique Quantique : de l'atome au solide

Physique statistique hors équilibre - examen

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Some informations are given in appendix

Subject : **Peierls instability in one-dimensional metals**

Introduction : Some metallic compounds are organised as weakly coupled one-dimensional (1D) chains. It is possible to show that the 1D metallic phase is unstable below a critical temperature T_{Peierls} under a periodic distorsion of the lattice with wavevector $q = 2k_F$, where k_F is the Fermi wavevector of the 1D metal : despite the cost in elastic energy, it is more favorable for the system to open a gap Δ at the Fermi level, what put the system in an *insulating* phase. At the same time the lattice distorsion induces a modulation of the electronic density called a *charge density wave*. It is the aim of the problem to study this metal-insulator transition from above ($T \geqslant T_{\text{Peierls}}$) by analysing the response of the electronic gas.

A. Compressibility of the 1D electronic gas.– We provide a **continuous description** of the electronic gas (we forget the lattice of atoms) : **electrons are free** and occupy usual 1D plane waves $\psi_k(x) = \frac{1}{\sqrt{L}}\mathrm{e}^{\mathrm{i}kx}$ of energy $\epsilon_k = \frac{k^2}{2m}$, with $k \in \mathbb{R}$ and where L is the length of the line (hence the wavevector is quantified). We set $\hbar = 1$. We will forget the spin and will treat electrons as **spinless fermions**.

1/ We consider the density operator for a *single electron* $\hat{n}(x)$ and its Fourier component $\hat{n}_q = \mathrm{e}^{-\mathrm{i}q\hat{x}}$, where $\hat{x}$ is the position operator for one electron. Give the matrix element $\langle \psi_k | \hat{n}_q | \psi_{k'} \rangle$.

2/ **Compressibility of the electron gas.**– Suppose that a perturbation is introduced under the form of a scalar external potential $V(x,t) = \frac{1}{L}\sum_q V_q(t)\mathrm{e}^{\mathrm{i}qx}$. The perturbation reads

$$\hat{H}_{\text{pert}}(t) = \int \mathrm{d}x\, V(x,t)\, \hat{n}(x) = \frac{1}{L}\sum_q V_q(t)\, \hat{n}_{-q}\,, \tag{1}$$

where $\hat{n}(x)$ is now the density of the electron gas. The compressibility characterizes its response :

$$\langle \hat{n}(x,t)\rangle_V = \langle \hat{n}(x)\rangle + \int \mathrm{d}t'\mathrm{d}x'\chi(x-x',t-t')\, V(x',t') + \mathcal{O}(V^2) \tag{2}$$

i.e. $\langle \hat{n}_q(t)\rangle_V = n\, L\, \delta_{q,0} + \int \mathrm{d}t'\widetilde{\chi}_q(t-t')\, V_q(t') + \mathcal{O}(V^2)$, where $n = \langle \hat{n}(x)\rangle$.

a) Express $\widetilde{\chi}_q(t)$ as an equilibrium correlation function.

b) Express its Fourier transform $\widetilde{\chi}(q,\omega) = \int \mathrm{d}t\, \widetilde{\chi}_q(t)\, \mathrm{e}^{\mathrm{i}\omega t}$ as a sum over contributions of plane waves. Analyse its analytical structure. Interpret the position of the poles of the integrand.

3/ **Static compressibility.**– In the rest of the problem we will consider the static response $\chi_T(q) \stackrel{\text{def}}{=} \widetilde{\chi}(q,0)$ at temperature T.

a) We denote $f_k \equiv f(\epsilon_k)$ the Fermi-Dirac distribution. Show that

$$\chi_T(q) = -\frac{1}{L}\sum_k \frac{f_k - f_{-k-q}}{\epsilon_{k+q} - \epsilon_k} = -\frac{2}{L}\sum_k \mathcal{PP}\frac{f_k}{\epsilon_{k+q} - \epsilon_k} \tag{3}$$

b) At zero temperature $T = 0$, we can use that $\frac{1}{L}\sum_k f_k \to \int_{-k_F}^{k_F} \frac{\mathrm{d}k}{2\pi}$, where $\epsilon_F = \frac{1}{2m}k_F^2$ is the Fermi energy. Compute explicitely $\chi_0(q)$.

c) Show that $\lim_{q\to 0}\chi_0(q)$ is related to the density of states at Fermi level $\rho_0 = \frac{m}{\pi k_F}$. Analyse $\chi_0(q)$ for $q \to 2k_F$ and $q \to \infty$. Plot carefully $\chi(q)/\rho_0$ as a function of $q/(2k_F)$.

4/ Static response at $q = 2k_F$ for finite T.– We assume that the chemical potential is independent on temperature, $\mu = \epsilon_F\ \forall\, T$. The divergence of $\chi_0(2k_F)$ originates from the neighbourhood of $k \sim -k_F$ in the sum (3). When $q \sim 2k_F$, it is therefore justified to linearize the spectrum as $\epsilon_k - \epsilon_F \simeq -v_F(k + k_F)$ and $\epsilon_{k+q} - \epsilon_F \simeq v_F(k + q - k_F)$, where $v_F = k_F/m$ is the Fermi velocity; hence we may simplify the sum in Eq. (3) as

$$\frac{1}{L}\sum_k \mathcal{PP}\frac{f_k}{\epsilon_{k+q} - \epsilon_k} \underset{q\sim 2k_F}{\longrightarrow} \int_{-k_F-k_c}^{-k_F+k_c} \frac{\mathrm{d}k}{2\pi}\, \frac{1}{\mathrm{e}^{\beta(\epsilon_k-\epsilon_F)} + 1}\, \frac{1}{\epsilon_{k+q} - \epsilon_k}\,, \tag{4}$$

where k_c is a cutoff (a scale over which the linearization of the spectrum is justified).

a) Compute $\chi_T(2k_F)$ for small temperatures $k_BT \ll \epsilon_c \overset{\text{def}}{=} v_Fk_c$ and deduce that the divergence of $\chi_0(2k_F)$ is regularized by thermal fluctuations (use integral given in the appendix).

b) Assuming that $\chi_T(q) \simeq \chi_0(q)$ far from $2k_F$ (when $\left|\frac{q}{2k_F} - 1\right| \gtrsim \frac{k_BT}{\epsilon_c}$), give a sketch of $\chi_T(q)$.

B. Coupling between electrons and lattice distorsions.– If $\delta n(x) = \langle \hat{n}(x)\rangle_V - n$ denotes the variation of density, the change in energy of the electron gas due to the introduction of the potential $V(x)$ can be expressed as

$$\delta E_{\text{elec}} = \frac{1}{L}\sum_q V_{-q}\,\delta n_q = \frac{1}{L}\sum_q \chi_T(q)\,|V_q|^2 \tag{5}$$

1/ Discuss the sign of δE_{elec}.

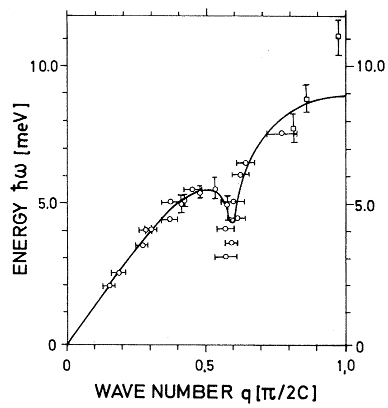

FIGURE 1 – *Kohn anomaly in the phonon spectrum of the quasi-1D conductor* $K_2Pt(CN)_4Br_{0.3}\cdot 3H_20$ *at* $T = 300\,\mathrm{K}$. *From : B. Renker et al, Phys. Rev. Lett.* **30**, *1144 (1973).*

The potential $V(x)$ is caused by a lattice distorsion characterised by some elastic energy E_{vib}. We consider a simple model of cristal : $N = L/a$ identical atoms of mass M with lattice spacing a. Elastic energy can be expressed in terms of the displacement of the n-th atom $\xi_n = \frac{1}{N}\sum_q \widetilde{\xi}_q \mathrm{e}^{\mathrm{i}qna}$

$$E_{\text{vib}} = \sum_{n=1}^{N} \frac{1}{2}M\omega_0^2\,(\xi_{n+1} - \xi_n)^2 = \frac{1}{N}\sum_q \frac{1}{2}M\omega_q^2\,|\widetilde{\xi}_q|^2 \tag{6}$$

where $\omega_q = 2\omega_0\,|\sin(qa/2)|$ is the phonon dispersion relation. Displacement of atoms is responsible for the potential « seen » by the electrons, therefore $\widetilde{\xi}_q$ and V_q are related. We assume :

$$V_q = \sqrt{\lambda\, a\, \frac{M}{2}}\, \omega_q\, \widetilde{\xi}_q\,, \tag{7}$$

where λ is a constant characterizing the electron-phonon coupling.

2/ Writing the total energy characterising the lattice distorsion as $\delta E_\mathrm{elec}+E_\mathrm{vib} = \frac{1}{N}\sum_q \frac{1}{2}M\Omega_q^2\,|\widetilde{\xi}_q|^2$, deduce the renormalised phonon dispersion relation Ω_q as a function of ω_q, λ and $\chi_T(q)$. Assuming weak coupling, $\lambda\rho_0 \ll 1$, give a sketch of Ω_q as a function of q for different temperatures. Discuss the experimental data (Fig. 1).

3/ Show that our approach can only be valid above a certain critical temperature, denoted T_Peierls. Express this temperature in terms of ϵ_c, λ and ρ_0. More difficult : interpret physically what occurs for $T = T_\mathrm{Peierls}$.

☞ Appendix :

• Convention for Fourier transform in dimension d :

$$f_q = \int_\mathrm{Vol} \mathrm{d}r\, \mathrm{e}^{-\mathrm{i}qr}\, f(r) \quad \& \quad f(r) = \frac{1}{\mathrm{Vol}}\sum_q f_q\, \mathrm{e}^{\mathrm{i}qr} \underset{\mathrm{Vol}\to\infty}{\longrightarrow} \int \frac{\mathrm{d}q}{(2\pi)^d} f_q\, \mathrm{e}^{\mathrm{i}qr} \tag{8}$$

• Consider two operators $\hat{A}$ and $\hat{B}$ sums of one-particle operators, as $\hat{A} = \sum_i \hat{a}^{(i)}$. If $\langle\cdots\rangle$ is the grand canonical averaging, we recall the useful relation

$$\big\langle[\hat{A}\,,\hat{B}]\big\rangle = \sum_\alpha f_\alpha\,\langle\,\varphi_\alpha\,|[\hat{a},\hat{b}]|\,\varphi_\alpha\,\rangle = \sum_{\alpha,\,\beta}(f_\alpha - f_\beta)\,a_{\alpha\beta}\,b_{\beta\alpha} \qquad \text{where } f_\alpha = \frac{1}{\mathrm{e}^{\beta(\epsilon_\alpha-\mu)}\pm 1} \tag{9}$$

and the summations run over individual (one-particle) stationary states. $a_{\alpha\beta} = \langle\,\varphi_\alpha\,|\hat{a}|\,\varphi_\beta\,\rangle$ is a matrix element of the one-body operator.
• We give the integral

$$\int_0^x \frac{\mathrm{d}y}{y}\tanh y \simeq \ln(\frac{4}{\pi}\mathrm{e}^{-\mathrm{C}}x) \qquad \text{for } x \gg 1 \tag{10}$$

where $\mathrm{C} = -0.577215...$ is the Euler-Mascheroni constant.

☞ More about quasi-1D conductors :

Beyond our simplified model : couplings between chains play a crucial role in order to stabilize the low temperature ordered phase (remember Mermin-Wagner theorem).
Few references :

• R. E. Peierls, Quantum theory of solids, Clarendon, Oxford, 1955.
• G. Grüner, Density waves in solids, Perseus, Cambridge, 1994.
• For a recent overview : P. C. Snijders & H. H. Weitering, *Electronic instabilities in self-assembled atom wires*, Rev. Mod. Phys. **82**, 307–329 (2010).

Solutions at `http://www.lptms.u-psud.fr/christophe_texier/`
(Cf. list of problems on the page of the course and section H.5 at the end of the notes).