Tutorial 5

1. Charge Screening and Thomas Fermi Approximation

a) Use the set of equations we established in the lecture in order to derive the general expression for the dielectric function

$$\epsilon(\boldsymbol{q}) = 1 - \frac{1}{\epsilon_0 q^2}\chi(\boldsymbol{q}) = 1 - \frac{1}{\epsilon_0 q^2}\frac{\rho^{ind}(\boldsymbol{q})}{\phi^{tot}(\boldsymbol{q})}$$

b) What are the assumptions made for the Thomas Fermi approximation?

c) Using these assumptions, one can write $\rho^{ind}(r) = -e\{n_0(\boldsymbol{r}) - n_0\}$, where n_0 is the homogeneous charge carrier concentration of the unperturbed system. Moreover, $n_0(\boldsymbol{r}) = n_0(\mu + e\phi^{tot}\{\boldsymbol{r}\})$, leading to

$$\rho^{ind}(r) = -e\{n_0(\mu + e\phi^{tot}\{\boldsymbol{r}\}) - n_0(\mu)\}$$

Show that

$$\epsilon(\boldsymbol{q}) = 1 + \frac{k_s^2}{q^2} \qquad \text{with} \qquad k_s = \sqrt{\frac{e^2}{\varepsilon_0}\frac{D(E_F)}{V}}$$

What happens for $q \to 0$?

[Hints: you can assume $e\phi^{tot} \ll \mu$ and use $\frac{D(E_F)}{V} = (\partial n_0/\partial\mu)_{\mu=E_F}$]

d) How large is the screening length $\lambda = 1/k_s$ for copper? How much for silicon? Compare them to the interatomic spacing.

2. Peierls Instability I

a) Describe in your own words: What is a Peierls instability and what are the ingredients?

b) In the lecture, we introduced the Lindhard response function

$$\chi(q) = \int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{f(\boldsymbol{k}) - f(\boldsymbol{k}+\boldsymbol{q})}{\varepsilon(\boldsymbol{k}) - \varepsilon(\boldsymbol{k}+\boldsymbol{q})} = \int \frac{d\boldsymbol{k}}{(2\pi)^d}\left(\frac{f(\boldsymbol{k})}{\varepsilon(\boldsymbol{k}+\boldsymbol{q}) - \varepsilon(\boldsymbol{k})} - \frac{f(\boldsymbol{k})}{\varepsilon(\boldsymbol{k}) - \varepsilon(\boldsymbol{k}-\boldsymbol{q})}\right)$$

Calculate $\chi(\boldsymbol{q})$ for 1 and 3 dimensions for a simple dispersion $\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{N_0\pi}{2L}\right)^2 = \frac{\hbar^2 k_F^2}{2m_e}$

[Hint: for the 1D case, assume a linear dispersion relation around the Fermi-energy $\varepsilon_k - \varepsilon_F = \hbar v_F(k - k_F)$]. Compare your result with the graph shown in the lecture. Assume low temperatures.

3. Peierls Instability II

a) In the lecture we introduced the reduced frequency of phonon modes

$$\omega_{ren,2k_F}^2 = \omega_{2k_F}^2 - \frac{g^2 n(\varepsilon_F)\omega_{2k_F}}{\hbar}\cdot ln\left(\frac{1.14\epsilon_0}{k_B T}\right)$$

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With $k_B T_{CDW} = 1.14\epsilon_0 e^{-1/\lambda}$ and the dimensionless electron phonon coupling $\lambda = \frac{g^2 n(\varepsilon_F)}{\hbar\omega_{2k_F}}$
Derive an expression of $\omega_{ren,2k_F}(T)$ slightly above T_{CDW}. What is the exponent?

b) The figure below shows a measurement of the phonon dispersion in ZrTe3 using inelastic X-Ray scattering [Original paper: Hoesch et al., PRL 102, 086402 (2009)]. What information can you deduce from the figure?

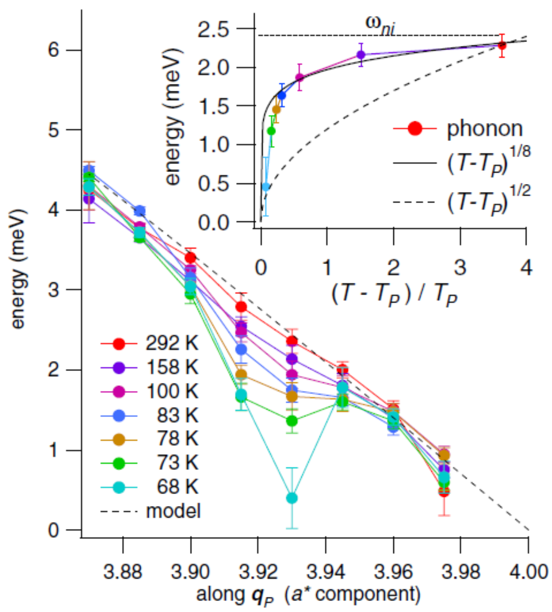

FIG. 2 (color online). Phonon dispersion from $(40\bar{1})$ in the direction of $\vec{q}_P$ at various temperatures $T > T_P$ above the transition. The inset shows the phonon energy $\hbar\omega_q$ at $\vec{q}_P$ as a function of reduced temperature $(T - T_P)/T_P$. The solid and dashed lines represent a 1/8 and a 1/2 power law, respectively.