Phonon Contribution to the Dynamic Form Factor of the Electrons in Metals

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For a metal a simple relation between the dynamical form factors $S_{\mathrm{el}}(\boldsymbol{q},\omega)$ and $S_{\mathrm{ion}}(\boldsymbol{q},\omega)$ is given for $\omega \ll q v_{\mathrm{f}}$ From this the phonon contribution to the electronic $\varepsilon(\boldsymbol{q},\omega)$ of a metal is derived. The relations are also valid in the presence of a static magnetic field. Here in special cases the phonon contributions can give spingularities in $\varepsilon(\boldsymbol{q},\omega,\boldsymbol{H})$.

Let us write the total electronic density of a metal

$$\varrho_{\mathrm{el}}(\boldsymbol{q},t)=\varrho_{\mathrm{el}}^{(0)}(\boldsymbol{q},t)+\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t) \tag{1}$$

where $\varrho_{\mathrm{el}}^{(0)}(\boldsymbol{q},t)$ shall describe the density fluctuations of the electrons in a rigid lattice.

$\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t)$ is the change due to all other effects, especially the lattice vibrations.

Forming the correlation function of (1) and taking the Fourier-transform of it, we get

$$S_{\mathrm{el}}(\boldsymbol{q},\omega)=S_{\mathrm{el}}^{0}(\boldsymbol{q},\omega)+\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}t\,e^{-i\omega t}$$
$$\times\left(\langle\Delta\varrho_{\mathrm{el}}(-\boldsymbol{q},0)\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t)\rangle+\langle\Delta\varrho_{\mathrm{el}}(-\boldsymbol{q},0)\varrho_{\mathrm{el}}^{(0)}(\boldsymbol{q},t)\rangle+\langle\varrho_{\mathrm{el}}^{(0)}(-\boldsymbol{q},0)\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t)\rangle\right) \tag{2}$$

where the dynamical structure factor is generally defined by

$$S(\boldsymbol{q},\omega):=\frac{1}{2\pi}\int\mathrm{d}t\,e^{-i\omega t}\langle\varrho(-\boldsymbol{q},0)\varrho(\boldsymbol{q},t)\rangle\,. \tag{3}$$

We want to consider (2) for $\omega \ll q v_{\mathrm{f}}$, i.e. for frequencies very small against typical electronic frequencies. Then the correlation functions under the integral have to be considered for times large against the electronic correlation time. For $t \gg \tau_{\mathrm{corr}}$ they can be factorized with respect to the electronic motion

$$\langle\Delta\varrho_{\mathrm{el}}(-\boldsymbol{q},0)\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t)\rangle+\langle\Delta\varrho_{\mathrm{el}}(-\boldsymbol{q},0)\varrho_{\mathrm{el}}^{(0)}(\boldsymbol{q},t)\rangle+\langle\varrho_{\mathrm{el}}^{(0)}(\boldsymbol{q},0)\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t)\rangle \tag{4}$$
$$\approx\langle\langle\Delta\varrho_{\mathrm{el}}(-\boldsymbol{q},0)\rangle_{\mathrm{el}}\langle\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t)\rangle_{\mathrm{el}}\rangle_{\mathrm{ion}}+\langle\Delta\varrho_{\mathrm{el}}(-\boldsymbol{q},0)\rangle\langle\varrho_{\mathrm{el}}^{(0)}(\boldsymbol{q},t)\rangle+\langle\varrho_{\mathrm{el}}^{(0)}(-\boldsymbol{q},0)\rangle\langle\Delta\varrho_{\mathrm{el}}(\boldsymbol{q},t)\rangle\,.$$

The second and third term on the r.h.s. of (4) do no longer depend on t. We are now going to approximate the first term.

Let us consider the vibrating ions of a metal as external charges that perturb the density of the conduction electrons. The linear response of the electrons to this perturbation is then given by

$$\langle\Delta\varrho_{\mathrm{el}}^{(1)}(\boldsymbol{q},\omega)\rangle_{\mathrm{el}}=\left(\frac{1}{\varepsilon_0(\boldsymbol{q},\omega)}-1\right)F(q)\,\Delta\varrho_{\mathrm{ion}}(\boldsymbol{q},\omega)\,. \tag{5}$$

Where $\varepsilon_0(\boldsymbol{q},\omega)$ is the dielectric function of the electron system if the lattice vibrations are absent. $F(q):=(-q^2/4\pi e^2)v(q)$ and $v(q)$ is the spacial Fourier-transform of the pseudopotential which is taken to describe the interaction between conduction electrons and ions.

$\Delta\varrho_{\mathrm{ion}}(\boldsymbol{q},\omega)$ is the Fourier-transform of the ion density change due to the displacement of the ions from their equilibrium positions $\boldsymbol{R}_{\mathrm{i}}^{0}$

$$\Delta\varrho_{\mathrm{ion}}(\boldsymbol{q},t):=\sum_i\left(\exp\{i\,\boldsymbol{q}\,\boldsymbol{R}_{\mathrm{i}}(t)\}-\exp\{i\,\boldsymbol{q}\,\boldsymbol{R}_{\mathrm{i}}^{0}\}\right)\,. \tag{6}$$

Approximating the first term on the r.h.s. of (4) with (5) we finally get for (2)

$$S_{\mathrm{el}}(\boldsymbol{q},\omega)=S_{\mathrm{el}}^{0}(\boldsymbol{q},\omega)+\left|\frac{1}{\varepsilon_0(\boldsymbol{q},\omega)}-1\right|^2|F(q)|^2\,S_{\mathrm{ion}}(\boldsymbol{q},\omega)+C(\boldsymbol{q})\,\delta(\omega)\,. \tag{7}$$

$C(\boldsymbol{q})$ results from the constant terms under the integral in (2). We need not know the difinite expression of it for further considerations.

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In (7) $S^0_{\text{el}}(\boldsymbol{q}, \omega)$ is the dynamical structure factor of the electrons in a rigid lattice. The second term gives the lowest order correction to $S_{\text{el}}(\boldsymbol{q}, \omega)$ caused by the lattice vibrations.

Using

$$\operatorname{Im} \frac{1}{\varepsilon(\boldsymbol{q}, \omega)} = \frac{4\pi^2 e^2}{q^2} \left[S_{\text{el}}(\boldsymbol{q}, \omega) - S_{\text{el}}(\boldsymbol{q}, -\omega)\right]. \tag{8}$$

(2) can be rewritten as a relation for the dielectric function of the electrons

$$\operatorname{Im} \varepsilon(\boldsymbol{q}, \omega) = \frac{|\varepsilon|^2}{|\varepsilon_0|^2} \left[\operatorname{Im} \varepsilon_0(\boldsymbol{q}, \omega) + \frac{4\pi^2 e^2}{q^2} |1 - \varepsilon_0(\boldsymbol{q}, \omega)^2 |F(q)|^2 (1 - e^{-\beta\omega}) S_{\text{ion}}(\boldsymbol{q}, \omega)\right]. \tag{9}$$

Expressions equivalent to (9) have been derived and discussed elsewhere[1]. We here want to show what may happen if a static magnetic field is present.

For the derivation of the above relations nothing will change except that all correlation functions and $\varepsilon_0(\boldsymbol{q}, \omega)$ have to be taken in the presence of the static magnetic field $\boldsymbol{H}$. So (9) is only replaced by the expression

$$\operatorname{Im} \varepsilon(\boldsymbol{q}, \omega, \boldsymbol{H}) = \frac{\varepsilon(\boldsymbol{q}, \omega, \boldsymbol{H})|^2}{\varepsilon_0(\boldsymbol{q}, \omega, \boldsymbol{H})|^2} \left[\operatorname{In} \varepsilon_0(\boldsymbol{q}, \omega, \boldsymbol{H}) + \frac{4\pi^2 e^2}{q^2} \cdot |1 - \varepsilon_0(\boldsymbol{q}, \omega, \boldsymbol{H})|^2 |F(q)|^2 (1 - e^{-\beta\omega}) S_{\text{ion}}(\boldsymbol{q}, \omega, \boldsymbol{H})\right]. \tag{9'}$$

In the case $\boldsymbol{H} = 0$ [1] we took the Ashcroft pseudopotential [2] for $F(q)$ and the Lindhard $\varepsilon(\boldsymbol{q}, \omega)$ [3] for $\varepsilon_0(\boldsymbol{q}, \omega)$ for a first discussion. We here take the same pseudopotential and $\varepsilon_0(\boldsymbol{q}, \omega, \boldsymbol{H})$ is approximated by the free electron function given by Blank and Kaner [4]. For a detailed discussion of it we refer to the original paper or to a paper of Cowley [5].

We here only discuss the case $\boldsymbol{H} \parallel \boldsymbol{q}$. Then $S_{\text{ion}}(\boldsymbol{q}, \omega, \boldsymbol{H}) \approx S_{\text{ion}}(\boldsymbol{q}, \omega, 0)$ [5] and the dielectric function is given by

$$\operatorname{Re} \varepsilon_{\text{BK}}(q, \omega, \boldsymbol{H}) = 1 + \frac{2 e^2 m^2 \omega_{\text{c}}}{\pi q^3} \sum \log \left| \frac{(K - 2x_n)^2 - \left(\dfrac{\omega}{K \varepsilon_{\text{F}}}\right)^2}{(K + 2x_n)^2 - \left(\dfrac{\omega}{K \varepsilon_{\text{F}}}\right)^2} \right|,$$

$$\operatorname{Im} \varepsilon_{\text{BK}}(q, \omega\, \boldsymbol{H}) = \frac{2 e^2 m^2 \omega_{\text{c}}}{\pi q^3} \alpha. \tag{10}$$

Here $K := q/k_{\text{f}}$ and $x_n{}^2 := 1 - (n + 1/2)\,\omega_{\text{c}}/\varepsilon_{\text{F}}$. N is the maximum value of n for which x_n is real. α is the number of integers which lie between

$$\frac{\varepsilon_{\text{F}}}{\omega_{\text{c}}} \left(1 - \frac{1}{4} \left(\frac{\omega}{K \varepsilon_{\text{F}}} - K\right)^2\right) \quad \text{and} \quad \frac{\varepsilon_{\text{F}}}{\omega_{\text{c}}} \left(1 - \frac{1}{4} \left(\frac{\omega}{K \varepsilon_{\text{F}}} + K\right)^2\right).$$

$\operatorname{Re} \varepsilon_{\text{BK}}(\boldsymbol{q}, \omega, \boldsymbol{H})$ has singularities when $\omega = \pm K \varepsilon_{\text{F}} (K + 2x_n)$ whereas the imaginary part remains finite. So it is evident from (9′) that there may appear singularities in $\operatorname{Im} \varepsilon(\boldsymbol{q}, \omega, \boldsymbol{H})$ because of the phonon contribution.

With the magnetic fields till now available the delta resonances in $\operatorname{Re} \varepsilon_{\text{BK}}(\boldsymbol{q}, \omega, \boldsymbol{H})$ are extremely close together, so that an experimental verification of them may be rather difficult.

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