

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

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(Z. Naturforsch. **30 a**, 109–110 [1975];
received September 16, 1974)

For a metal a simple relation between the dynamical form factors $S_{\text{el}}(\mathbf{q}, \omega)$ and $S_{\text{ion}}(\mathbf{q}, \omega)$ is given for $\omega \ll q v_f$. From this the phonon contribution to the electronic

$\varepsilon(\mathbf{q}, \omega)$ 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 singularities in $\varepsilon(\mathbf{q}, \omega, \mathbf{H})$.

Let us write the total electronic density of a metal

$$\varrho_{\text{el}}(\mathbf{q}, t) = \varrho_{\text{el}}^{(0)}(\mathbf{q}, t) + \Delta\varrho_{\text{el}}(\mathbf{q}, t) \quad (1)$$

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

$\Delta\varrho_{\text{el}}(\mathbf{q}, t)$ 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

$$S_{\text{el}}(\mathbf{q}, \omega) = S_{\text{el}}^0(\mathbf{q}, \omega) + \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-i\omega t} \times (\langle \Delta\varrho_{\text{el}}(-\mathbf{q}, 0) \Delta\varrho_{\text{el}}(\mathbf{q}, t) \rangle + \langle \Delta\varrho_{\text{el}}(-\mathbf{q}, 0) \varrho_{\text{el}}^{(0)}(\mathbf{q}, t) \rangle + \langle \varrho_{\text{el}}^{(0)}(-\mathbf{q}, 0) \Delta\varrho_{\text{el}}(\mathbf{q}, t) \rangle) \quad (2)$$

where the dynamical structure factor is generally defined by

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

We want to consider (2) for $\omega \ll q v_f$, 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 $t \gg \tau_{\text{corr}}$ they can be factorized with respect to the electronic motion

$$\langle \Delta\varrho_{\text{el}}(-\mathbf{q}, 0) \Delta\varrho_{\text{el}}(\mathbf{q}, t) \rangle + \langle \Delta\varrho_{\text{el}}(-\mathbf{q}, 0) \varrho_{\text{el}}^{(0)}(\mathbf{q}, t) \rangle + \langle \varrho_{\text{el}}^{(0)}(\mathbf{q}, 0) \Delta\varrho_{\text{el}}(\mathbf{q}, t) \rangle \quad (4)$$

$$\approx \langle \langle \Delta\varrho_{\text{el}}(-\mathbf{q}, 0) \rangle_{\text{el}} \langle \Delta\varrho_{\text{el}}(\mathbf{q}, t) \rangle_{\text{el}} \rangle_{\text{ion}} + \langle \Delta\varrho_{\text{el}}(-\mathbf{q}, 0) \rangle \langle \varrho_{\text{el}}^{(0)}(\mathbf{q}, t) \rangle + \langle \varrho_{\text{el}}^{(0)}(-\mathbf{q}, 0) \rangle \langle \Delta\varrho_{\text{el}}(\mathbf{q}, t) \rangle.$$

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

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

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

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

$$\Delta\varrho_{\text{ion}}(\mathbf{q}, t) := \sum_i (\exp\{i\mathbf{q} \cdot \mathbf{R}_i(t)\} - \exp\{i\mathbf{q} \cdot \mathbf{R}_i^0\}). \quad (6)$$

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

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

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

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

Using

$$\text{Im} \frac{1}{\varepsilon(\mathbf{q}, \omega)} = \frac{4\pi^2 e^2}{q^2} [S_{el}(\mathbf{q}, \omega) - S_{el}(\mathbf{q}, -\omega)]. \quad (8)$$

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

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

Expressions equivalent to (9) have been derived and discussed elsewhere¹. 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 $\varepsilon_0(\mathbf{q}, \omega)$ have to be taken in the presence of the static magnetic field $\mathbf{H}$. So (9) is only replaced by the expression

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

In the case $\mathbf{H}=0$ ¹ we took the Ashcroft pseudopotential² for $F(q)$ and the Lindhard $\varepsilon(\mathbf{q}, \omega)$ ³ for $\varepsilon_0(\mathbf{q}, \omega)$ for a first discussion. We here take the same pseudopotential and $\varepsilon_0(\mathbf{q}, \omega, \mathbf{H})$ is approximated by the free electron function given by Blank and Kaner⁴. For a detailed discussion of it we refer to the original paper or to a paper of Cowley⁵.

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

$$\begin{aligned} \text{Re} \varepsilon_{BK}(q, \omega, \mathbf{H}) &= 1 + \frac{2e^2 m^2 \omega_c}{\pi q^3} \sum \log \left| \frac{(K - 2x_n)^2 - \left(\frac{\omega}{K \varepsilon_F}\right)^2}{(K + 2x_n)^2 - \left(\frac{\omega}{K \varepsilon_F}\right)^2} \right|, \\ \text{Im} \varepsilon_{BK}(q, \omega, \mathbf{H}) &= \frac{2e^2 m^2 \omega_c}{\pi q^3} \alpha. \end{aligned} \quad (10)$$

Here $K := q/k_t$ and $x_n^2 := 1 - (n + 1/2)\omega_c/\varepsilon_F$. N is the maximum value of n for which x_n is real. α is the number of integers which lie between

$$\frac{\varepsilon_F}{\omega_c} \left(1 - \frac{1}{4} \left(\frac{\omega}{K \varepsilon_F} - K \right)^2 \right) \quad \text{and} \quad \frac{\varepsilon_F}{\omega_c} \left(1 - \frac{1}{4} \left(\frac{\omega}{K \varepsilon_F} + K \right)^2 \right).$$

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

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

Acknowledgements

The author thanks the Deutsche Forschungsgemeinschaft for enabling him a long stay at Kiev State University.

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³ J. Lindhard, Mat. Fys. Medd. **28**, 8 [1954].

⁴ A. Ya. Blank and E. A. Kaner, Soviet Physics JETP **23**, 673 [1966].

⁵ R. A. Cowley, Conference Proceedings 1968, Inelastic Scattering of Neutrons in Solid and Liquids, Vienna: IAEA.