The sign of the static dielectric constant of simple metals

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(Submitted 24 March 1978)
Pis'ma Zh. Eksp. Teor. Fiz. **28**, No. 1, 3–6 (5 July 1978)

It is shown that the static dielectric constant $\epsilon(\mathbf{q},0)$ of simple metals can have negative values. This circumstance is due to the large negative contribution of the pointlike ions to the polarizability of the metal.

PACS numbers: 77.20.+y

1. It is known[1] that the Fourier component of the interaction of two charges in a medium can be expressed with the aid of the dielectric constant of this medium $\epsilon(\mathbf{q}, \omega)$

$$V(\mathbf{q}, \omega) = \frac{4\pi e^2}{q^2 \epsilon(\mathbf{q}, \omega)} . \tag{1}$$

Under certain assumptions (for details see the monograph[1]) the effective interelectron interaction in metals can also be written in the form (1). In this case $\epsilon(\mathbf{q}, \omega)$ is the total dielectric constant of the metal and includes the polarizabilities of both the electron and the ion subsystems.

The total interelectron interaction consists of direct Coulomb repulsion, with a constant μ, and an effective attraction due to phonon (exciton) exchange, with a coupling constant λ. It was shown in[2,3] that a simple connection exists between the constants μ and λ:

$$\mu - \lambda = N(0) \int_0^{2k_F} dq / q \epsilon(\mathbf{q}, \omega) . \tag{2}$$

2. The effective interelectron interaction influences substantially many properties of metals, and in particular the critical temperature T_c of the superconducting transition.

Formulas relating the values of T_c with the constants μ and λ were derived in[2]. It was shown[2,3] that very substantial limitations appear on the possible maximal values of T_c if the Coulomb constant μ in the metal exceeds λ. As seen from (2), the ratio of the quantities μ and λ is completely determined by the sign of the static dielectric constant $\epsilon(\mathbf{q},0)$.

3. The question of the sign of the static dielectric constant of a medium has been discussed repeatedly.[3–5] In particular, it is stated in the book by Pines and Nozieres[4]

that the condition $\epsilon(\mathbf{q},0)>0$ is the stability criterion of the system relative to formation of charge density waves (CDW). Kirzhnits[5] has shown, however, that the actual condition for the stability of the system to CDW formation is either $\epsilon(\mathbf{q},0)>1$ or $\epsilon(\mathbf{q},0)<0$. The possible existence of systems with negative dielectric constant has thus been proven. Kirzhnits,[5] however, left open the question of the real existence of such media. We show in the present paper that systems with negative dielectric constants really exist in nature and are in no way exotic. In particular, it will be shown that simple metals can serve as examples of a system in which $\epsilon(\mathbf{q},0)<0$.

The reciprocal dielectric constant of a metal $\epsilon^{-1}(x,x')$, as shown in[1,6], can be written in the form:

$$\epsilon^{-1}(x, x_1) = \epsilon_{el}^{-1}(x, x_1) + \sum_{n,n'} \int dx_2\, dx_3\, \epsilon_{el}^{-1}(x, x_2)\, \nabla_{\alpha} \Phi(\mathbf{r}_2 - \mathbf{R}_n^0) \times D_{nn'}^{\alpha\beta}(t_2 - t_3)\, \nabla_{\beta} \Phi(\mathbf{r}_3 - \mathbf{R}_{n'}^0)\, \frac{\nabla_{\mathbf{r}_3}^2}{4\pi e^2}\, \epsilon_{el}^{-1}(x_3, x_1). \tag{3}$$

In this formula $\epsilon_{el}^{-1}(x,x')$ is the reciprocal dielectric constant of electrons in a rigid lattice, $\Phi(\mathbf{r}-\mathbf{R}_n^0)$ is the pseudopotential of the interaction of an electron with an ion at the point $\mathbf{R}_n^0$ and $D_{nn'}^{\alpha\beta}(t)$ is the Green's function of the ion displacements.

On going to momentum space, the function $\epsilon^{-1}(x,x')$ is transformed into a matrix $\epsilon^{-1}(\mathbf{q}+\mathbf{K}, \mathbf{q}+\mathbf{K}', \omega)$ in the reciprocal-lattice vectors $\mathbf{K}$ and $\mathbf{K}'$. We confine ourselves henceforth to the diagonal element $\epsilon^{-1}(\mathbf{q}+0,\mathbf{q}+0,\omega)$. It is known[7] that the macroscopic dielectric constant of the system $\epsilon(\mathbf{q},\omega)$ is expressed in terms of the function

$$\epsilon(\mathbf{q}, \omega) = 1/\epsilon^{-1}(\mathbf{q}+0, \mathbf{q}+0, \omega). \tag{4}$$

4. For simple metals we can neglect entirely[1] the off-diagonal matrix elements $\epsilon_{el}^{-1}(\mathbf{q}+\mathbf{K},\mathbf{q}+\mathbf{K}',\omega)$ with $\mathbf{K}\neq\mathbf{K}'\neq 0$. In this case, going over to the momentum representation, we can express the macroscopic dielectric constants for the high-symmetry directions in the form:

$$1/\epsilon(\mathbf{q},0) = \frac{1}{\epsilon_{el}(\mathbf{q},0)} \left[1 - \frac{\Omega_{pl}^2}{\epsilon_{el}(\mathbf{q},0)\,\omega_{\parallel}^2(\mathbf{q})} \left(\frac{\Phi(\mathbf{q})}{V_c(\mathbf{q})}\right)^2\right], \tag{5}$$

where $\Omega_{pl}=\sqrt{4\pi Z^2 e^2 N/M}$ is the ion plasma frequency, $\omega_{\parallel}(\mathbf{q})$ is the frequency of the longitudinal phonons, and $V_c(\mathbf{q})=4\pi Ze^2/q^2$ is the ion Coulomb potential.

In the isotropic structureless "jellium" model, where $\Phi(\mathbf{q})=V_c(\mathbf{q})$ and

$\omega_{\parallel}^2(\mathbf{q})=\Omega_{pl}^2/\epsilon_{el}(\mathbf{q},0)$, the electron and ion contributions cancel each other completely, and $1/\epsilon(\mathbf{q},0)=0$ at all momenta $\mathbf{q}$. The situation is entirely different in a crystal, where transverse ion oscillations are present in addition to the longitudinal ones.

In particular, for a Coulomb system (for example, metallic Hydrogen), where $V_c(\mathbf{q})\equiv\Phi(\mathbf{q})$, we can write the sum rule

$$\omega_{\parallel}^2(\mathbf{q}) = \frac{\Omega_{pl}^2}{\epsilon_{el}}(\mathbf{q},0) - \sum_{\lambda_\perp}\omega_\perp^2(\mathbf{q}) + \sum_{\mathbf{K}\neq 0}\left[\frac{1}{\epsilon_{el}}(\mathbf{q}+\mathbf{K},0) - \frac{1}{\epsilon_{el}}(\mathbf{K},0)\right]. \qquad (6)$$

We see therefore that the situation $\omega_{\parallel}^2(\mathbf{q})<\Omega_{pl}^2/\epsilon_{el}(\mathbf{q},0)$ is already perfectly feasible in a crystal. In this case it is obvious from (5) that the macroscopic dielectric constant of such a crystal is negative. Calculations of $\epsilon(\mathbf{q},0)$ for metallic hydrogen using the calcu-

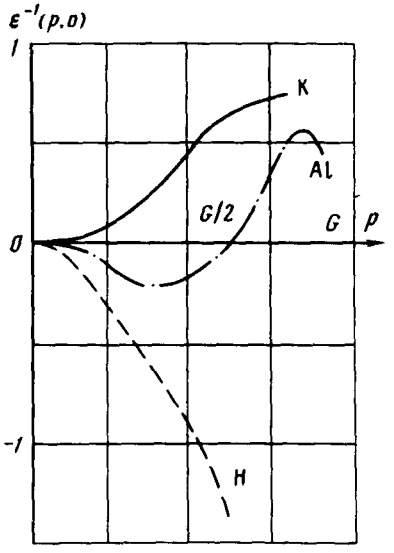

FIG. 1. Total reciprocal macroscopic dielectric constants of Al and K and of metallic hydrogen ($r_s=1$, fcc lattice). $\mathbf{p}$ is the momentum in the expanded Brillouin zone in the (1,0,0) direction ($\mathbf{G}$ is the nearest reciprocal-lattice vector in this direction).

lated $\omega_\lambda(\mathbf{q})$ from[8] are shown in Fig. 1. It is seen that in metallic hydrogen $\epsilon(\mathbf{q},0)$ is negative at all values of $\mathbf{q}$.

For simple metals, where the electron-ion pseudopotential is not pure-Coulomb, various situations are possible, depending on the relation between $\Phi(\mathbf{q})$ and $V_c(\mathbf{q})$. Calculations of the dielectric constants of K and Al, using the real phonon spectra and pseudopotentials of these metals,[9] are also shown in Fig. 1.

We see thus that $\epsilon(\mathbf{q},0)$ of simple metal can have any sign, including negative. This circumstance is due mainly to the strong polarizability of pointlike ions. We shall not concern ourselves here with problems connected with the influence of negative $\epsilon(\mathbf{q},0)$ on the superconductivity of a metal.

In conclusion, the authors are sincerely grateful to D.A. Kirzhnits and V.L. Ginzburg for interest in the work and for help.

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