Fano resonance in a system of interacting electrons and phonons

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(Submitted 6 July 1995)
Pis'ma Zh. Éksp. Teor. Fiz. **62**, No. 3, 227–230 (10 August 1995)

Raman scattering with excitation of a phonon is studied under conditions where the scattering is due to the interaction of light with the conduction electrons. The line has the shape of a Fano antiresonance. The screening of the electron-photon coupling and of the deformation potential as a result of the Coulomb interaction of the electrons is taken into account. The parameters of the 350 cm^{-1} line and the electron-phonon constant in superconducting YBaCuO are estimated by comparing with experiment. © *1995 American Institute of Physics.*

1. A narrow resonance observed against the background of a diffuse continuum is commonly referred to as a Fano resonance. Here we shall study the resonance in inelastic scattering of light in metals with the excitation or absorption of a phonon. The corresponding continuum is associated with the scattering of light by electron-hole pairs. If the electron-phonon interaction is taken into account, then the narrow resonance loses its Lorentzian shape. The asymmetric shape of the line is a characteristic indicator of a Fano resonance. Such lines are often observed in experiments[1–3] and there exist several theories[4–6] which explain their shape.

Ordinarily, the quantum-mechanical approach is used and a very simple case in which the spatial dispersion can be ignored, is considered. However, the corresponding condition $kv \ll |\omega + i/\tau|$ ($v \simeq 10^8$ cm/s is the Fermi velocity, τ^{-1} is the electron collision frequency, and k and ω are the characteristic wave vector and frequency) is by no means always satisfied, for example, as in the case of the scattering of light with the wave vector $k \simeq \omega_p/c$, where $\omega_p \simeq 3\times 10^{15}$ s^{-1} is the plasma frequency of the electrons. If an optical phonon with frequency ω_D is excited in the process, then the collision frequency is

$$\tau^{-1} \simeq 2\pi g \ \max(\omega_D, T), \tag{1}$$

where the Debye frequency is $\omega_D \simeq 3\times 10^{13}$ s^{-1}. Setting the dimensionless electron-phonon coupling constant $g \sim 0.5$ (we shall discuss this value below), we see that both weak and strong spatial dispersions are possible.

In Ref. 6, where this problem was studied in the long-wavelength limit, the method of Green's functions was employed. This is an unjustifiably complicated approach, since the transferred wave vector $\mathbf{k} = \mathbf{k}^{(i)} - \mathbf{k}^{(s)}$ and frequency $\omega = \omega^{(i)} - \omega^{(s)}$ (the indices i and s denote the corresponding values of the incident and scattered light in the sample) are small compared to the Fermi momentum and energy, and to calculate the response, whose

imaginary part represents the differential scattering cross section, it is simpler to use the classical kinetic equation.[7,8]

2. We shall calculate the response of the electronic system, which interacts with phonons, to a disturbance $\gamma(\mathbf{p})U(\mathbf{k},\omega)$, where $\gamma(\mathbf{p})=e_\alpha^{(i)}\gamma_{\alpha\beta}(\mathbf{p})e_\alpha^{(s)}$ is bilinear in the polarization vectors of the incident and scattered light, and $\gamma_{\alpha\beta}(\mathbf{p})$ takes into account both intra- and interband virtual transitions.[9]

Taking into consideration the interaction of electrons with the field $U(\mathbf{k},\omega)$ and with the acoustic $u(\mathbf{k},\omega)$ and optical $w(\mathbf{k},\omega)$ oscillations, we write the change in the electronic energy as

$$\varepsilon(\mathbf{p},\mathbf{k},\omega)=\varepsilon_0(\mathbf{p})+\gamma(\mathbf{p})U(\mathbf{k},\omega)+\lambda_{jk}(\mathbf{p})u_{jk}(\mathbf{k},\omega)+\xi_j(\mathbf{p})w_j(\mathbf{k},\omega), \tag{2}$$

where $\lambda_{jk}(\mathbf{p})$ and $\xi_j(\mathbf{p})$ are the corresponding deformation potential and displacement field.

It can be shown[8] that the Coulomb interaction of the electrons and the "collisional" part of their interaction with the impurities and phonons screen all bare vertices so that the following substitutions must be made:

$$\gamma(\mathbf{p})\to\gamma(\mathbf{p})-\langle\gamma(\mathbf{p})\rangle/\langle 1\rangle,\quad \lambda_{ik}(\mathbf{p})\to\lambda_{ik}(\mathbf{p})-\langle\lambda_{ik}(\mathbf{p})\rangle/\langle 1\rangle,$$
$$\xi_i(\mathbf{p})\to\xi_i(\mathbf{p})-\langle\xi_i(\mathbf{p})\rangle/\langle 1\rangle, \tag{3}$$

where the brackets indicate integration over the Fermi surface. After such a substitution, the Coulomb interaction can be disregarded up to frequencies $\omega<\omega_p$, and the collision integral can be written in the relaxation-time approximation.

Solving the kinetic equation, we obtain for the electron distribution function

$$f_p(\mathbf{k},\omega)=f_0(\varepsilon_0)+\Pi[(\mathbf{v}\cdot\mathbf{k},\omega)][\varepsilon(\mathbf{p},\mathbf{k},\omega)-\varepsilon_0(\mathbf{p})]\frac{df_0}{d\varepsilon_0}, \tag{4}$$

where

$$\Pi(\mathbf{v}\cdot\mathbf{k},\omega)=\frac{i\tau^{-1}-\mathbf{v}\cdot\mathbf{k}}{\omega+i\tau^{-1}-\mathbf{v}\cdot\mathbf{k}}, \tag{5}$$

and f_0 is the Fermi function. Substituting this expression into the equation of motion for the phonons, for example, optical phonons, we obtain

$$[\omega^2(\mathbf{k})-\omega^2-\Gamma(\mathbf{k},\omega)]w(\mathbf{k},\omega)=\frac{1}{\rho}\langle\gamma(\mathbf{p})\xi(\mathbf{p})\Pi(\mathbf{v}\cdot\mathbf{k},\omega)\rangle U(\mathbf{k},\omega), \tag{6}$$

where

$$\Gamma(\mathbf{k},\omega)=\frac{1}{\rho}\langle\xi^2(\mathbf{p})\Pi(\mathbf{v}\cdot\mathbf{k},\omega)\rangle, \tag{7}$$

ρ is the reduced mass of a unit cell, and for brevity we drop the vector indices, making the assumption that an oscillation with frequency $\omega(\mathbf{k})$ is not coupled with other oscillations. The real part of Γ describes the frequency shift and the imaginary part describes the damping of the optical phonons.

The expressions (4)–(7) make it possible to calculate the response $\chi(\mathbf{k},\omega)$ to the perturbation $\gamma(\mathbf{p})U(\mathbf{k},\omega)$. Using the definition

$$\int \frac{2d^3p}{(2\pi)^3}\gamma(\mathbf{p})[f_p(\mathbf{k},\omega)-f_0(\varepsilon_0)]=-\chi(\mathbf{k},\omega)U(\mathbf{k},\omega),$$

we find

$$\chi(\mathbf{k},\omega)=\langle\gamma^2(\mathbf{p})\Pi(\mathbf{v}\cdot\mathbf{k},\omega)\rangle-\frac{\langle\gamma(\mathbf{p})\xi(\mathbf{p})\Pi(\mathbf{v}\cdot\mathbf{k},\omega)\rangle^2}{\rho[\omega^2(\mathbf{k})-\omega^2-\Gamma(\mathbf{k},\omega)]}. \tag{8}$$

The first term in Eq. (8) represents the contribution of electron-hole excitations. Its imaginary part, which determines the cross section for inelastic scattering of light, has the following form in the limiting cases of weak and strong spatial dispersion:

$$\chi''_{eh}(\mathbf{k},\omega)=\frac{\omega\tau}{(\omega\tau)^2+1}\langle\gamma^2(\mathbf{p})\rangle \quad \text{for } kv\ll|\omega+i/\tau|, \tag{9}$$

$$\chi''_{eh}(\mathbf{k},\omega)=(\pi\omega/k)\langle\gamma^2(\mathbf{p})\delta(\nu)/v\rangle \quad \text{for } kv\gg|\omega+i/\tau|, \tag{10}$$

where $\cos\nu=\mathbf{k}\cdot\mathbf{v}/kv$, and $\delta(\nu)$ is a Dirac delta function. We underscore that the subtraction (3) must be made in Eqs. (8)–(10).

The second term is the resonance at the frequency $\omega(\mathbf{k})$. It is easy to see that the sign of the imaginary part of this term can be different from that of the imaginary part of the electron-hole contribution, and they have a positive sign only in the sum, as should be the case. Separating the imaginary part (8), we find for $kv\ll|\omega+i/\tau|$:

$$\chi''(\mathbf{k},\omega)=\chi''_{eh}(\mathbf{k},\omega)\frac{[\omega^2(\mathbf{k})-\Gamma'+\omega_0^2-\omega^2]^2+A^2}{[\omega^2(\mathbf{k})-\Gamma'-\omega^2]^2+\Gamma''^2}, \tag{11}$$

where $\chi''_{eh}(\mathbf{k},\omega)$ is given by Eq. (9),

$$\Gamma=\frac{1}{\rho}\langle\xi^2(\mathbf{p})\rangle\frac{1+i\omega\tau}{(1+\omega^2\tau^2)}, \tag{12}$$

$$\omega_0^2=\frac{\langle\xi(\mathbf{p})\gamma(\mathbf{p})\rangle^2}{\rho\langle\gamma^2(\mathbf{p})\rangle(1+\omega^2\tau^2)}, \tag{13}$$

$$A^2=\left(\langle\xi^2(\mathbf{p})\rangle-\frac{\langle\xi(\mathbf{p})\gamma(\mathbf{p})\rangle^2}{\langle\gamma^2(\mathbf{p})\rangle}\right) \tag{14}$$

$$\times\left(\frac{\langle\xi(\mathbf{p})\gamma(\mathbf{p})\rangle^2}{\langle\gamma^2(\mathbf{p})\rangle}+\langle\xi^2(\mathbf{p})\rangle\omega^2\tau^2\right)\rho^{-2}(1+\omega^2\tau^2)^{-2}.$$

In the short-wavelength limit $kv\gg|\omega+i/\tau|$ we obtain an expression of the type (11), where $\chi''_{eh}(\mathbf{k},\omega)$ is given by Eq. (10), and all other symbols are defined as follows:

$$\Gamma=\frac{1}{\rho}\left(\langle\xi^2(\mathbf{p})\rangle+i\pi\frac{\omega}{k}\langle\xi^2(\mathbf{p})\delta(\nu)/v\rangle\right), \tag{15}$$

$$\omega_0^2=\frac{\langle\xi(\mathbf{p})\gamma(\mathbf{p})\rangle\langle\xi(\mathbf{p})\gamma(\mathbf{p})\delta(\nu)/v\rangle}{\rho\langle\gamma^2(\mathbf{p})\delta(\nu)/v\rangle}, \tag{16}$$

$$A^2=[\langle\xi^2(\mathbf{p})\delta(\nu)/v\rangle\langle\gamma^2(\mathbf{p})\delta(\nu)/v\rangle-\langle\xi(\mathbf{p})\gamma(\mathbf{p})\delta(\nu)/v\rangle^2] \tag{17}$$

$$\times\frac{\langle\xi(\mathbf{p})\gamma(\mathbf{p})\rangle^2}{\rho^2\langle\gamma^2(\mathbf{p})\delta(\nu)/v\rangle^2}.$$

We note that the imaginary part Γ'' is proportional to the frequency. Taking into account the damping (if it is small) and the shift, which are attributable to the interaction with electrons, we can write the phonon spectrum in the form

$$\omega=\tilde{\omega}(\mathbf{k})-i\Gamma''/2\omega,\quad \tilde{\omega}^2(\mathbf{k})=\omega^2(\mathbf{k})-\Gamma'.$$

3. The second factor in Eq. (11) describes an asymmetric resonance: There is a maximum, which in the case of small Γ'' lies at $\tilde{\omega}(\mathbf{k})$, and a minimum at $\omega_{\min}$, which is determined by the condition $\omega_{\min}^2=\tilde{\omega}^2(\mathbf{k})+\omega_0^2+A^2/\omega_0^2$. The minimum thus lies at a higher frequency than the maximum, and this is seen especially clearly in superconducting YBaCuO (Refs. 2 and 3) on the two antiresonances at 115 cm^{-1} and 350 cm^{-1}. In our case a nonzero A is obtained only as a result of the momentum dependence of the vertices $\gamma(\mathbf{p})$ and $\xi(\mathbf{p})$. For $A=0$ the scattering cross section vanishes at some transferred frequency. In general, a nonzero A can also be obtained by taking into account the scattering of light by the phonons themselves — this scattering appears, for example, in a dielectric as a result of fluctuations of the permittivity and it can be described at the microscopic level in terms of virtual transitions of electrons from completely filled bands into unoccupied bands. This situation was studied in Ref. 6, where a nonzero A is obtained only as a result of the characteristic damping of the phonons. Equation (11) then becomes much more complicated (we shall give this equation in a detailed paper) — two additional constants appear. It would make sense to discuss it here, if experimental data existed on Raman scattering with a transition from metallic to dielectric samples.

Using Eqs. (11)–(14), we described the shape of the resonance line[3] with $\omega^*=350$ cm^{-1} in YBaCuO and we determined the values of the constants as $\Gamma''/2\omega^*=13$ cm^{-1}, $\omega_0\simeq\sqrt{A}=120$ cm^{-1}, $\omega^*\tau=0.30$. Using Eq. (1), we estimated the electron-phonon constant as $g=0.53$, setting $\omega_D=\omega^*$. Of course, for YBaCuO a suitable value for the Debye temperature is 500 K. It is also doubtful that taking into account the characteristic scattering, which was discussed above, can change the value of g substantially, since the line is strongly asymmetric.

The analysis presented here is also applicable to (Mandel'shtam) Brillouin scattering, i.e. scattering with excitation of an acoustic phonon — it is only necessary to make the substitution $\xi\to k\lambda$ in Eqs. (11)–(17).

In conclusion, we wish to make the following remark concerning the distribution of the incident radiation in the metal. The formulas presented above refer to the case in which the damping of this field is weak compared to the phonon damping, and as the transferred wave vector $\mathbf{k}$ we must use the doubled wave vector of the incident radiation in the metal (for the backscattering geometry). This condition is stated explicitly in Ref. 8 in the derivation of Eq. (52).

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Translated by M. E. Alferieff