

Proceedings of the European Conference "Physics of Magnetism 96", Poznań 1996

FANO RESONANCE IN A COUPLED ELECTRON-PHONON SYSTEM

L.A. FALKOVSKY

Landau Institute for Theoretical Physics, Russian Academy of Sciences
Kosygina 2, 117 334 Moscow, Russia

AND S. KLAMA

Institute of Molecular Physics, Polish Academy of Sciences
Smoluchowskiego 17, 60-179 Poznań, Poland

Raman light scattering with excitation of electron-hole continuum and a phonon is investigated theoretically. The effect of a surface and 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 340 cm^{-1} resonance line in superconducting YBaCuO are estimated by comparing with experimental data.

PACS numbers: 73.20.Mf, 74.25.-q, 78.30.-j

1. Introduction

We study the resonance in inelastic light scattering in metals with the excitation of electron-hole pairs continuum and a phonon. If the electron-phonon interaction is taken into account, the narrow resonance loses its Lorentzian shape. The asymmetric shape of the line is a characteristic indicator of the Fano resonance or the Breit-Wigner line 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 $kv \ll |\omega + i/\tau|$ ($v \approx 10^8 \text{ cm/s}$ is the Fermi velocity, τ^{-1} is the electron collision rate, and k and ω are the characteristic wave vector and frequency) is by no means always satisfied, for example in the case of the scattering of light with the wave vector $k \approx \omega_p/c$, where $\omega_p \approx 3 \times 10^{15} \text{ s}^{-1}$ is the plasmon frequency. If an optical phonon with frequency ω_D is excited in the process, the collision rate $\tau^{-1} \approx 2\pi g_{ep} \max(\omega_D, T)$, $\omega_D \approx 3 \times 10^{13} \text{ s}^{-1}$. Setting the electron-phonon coupling constant $g_{ep} \approx 0.5$, we see that both weak and strong spatial dispersions are possible.

If the transferred wave vector $\mathbf{k} = \mathbf{k}^{(i)} - \mathbf{k}^{(s)}$ and frequency $\omega = \omega^{(i)} - \omega^{(s)}$ ((i) stands for incident, (s) for scattered light in metal) are small compared to the

Fermi momentum and energy, respectively, the classical kinetic equation for the electrons and equation of motion for phonons with appropriate boundary conditions can be applied to calculate the response, whose imaginary part represents the differential light scattering cross-section (LSCS) [1, 2]. The effective Hamiltonian describing the interactions in the considered system has the following form:

$$\hat{\mathcal{H}} = \frac{e^2}{mc^2} \int d^3r \tilde{\mathcal{N}}(r, t) U(r, t), \quad (1)$$

where $\tilde{\mathcal{N}}(r, t) = \int \frac{d^3p}{(2\pi)^3} \gamma(p) \hat{f}_p(r, t) + g_{ik}^{ac} u_{ik}(r, t) + g_i^{opt} w_i(r, t)$ and $\hat{f}_p(r, t)$ is the electronic density fluctuation operator, $u_{ik}(r, t)$ is the deformation tensor, w_i is the displacement corresponding to the optical phonons; and $\gamma(p)$, g_{ik}^{ac} , and g_i^{opt} are the vertex functions containing resonance denominators (for $\omega^{(i)}$ or $\omega^{(s)}$ equal to interband transition frequencies) appearing in the second order of the perturbation theory with respect to vector potentials of the incident $A^{(i)}(r, t)$ and scattered $A^{(s)}(r, t)$ light. It can be shown [2] that the Coulomb interaction of the electrons and the "collisional" part of their interaction with the impurities and phonons screen all bare vertices $\gamma(p)$, $\xi_i(p)$, $\lambda_{ik}(p)$ so that the substitutions like $\gamma(p) \rightarrow \gamma(p) - \langle \gamma(p) \rangle / \langle 1 \rangle$ must be made, where $\langle (\dots) \rangle$ denotes the integration over the Fermi surface; $i, k = x, y, z$; $U(r, t) \approx A^{(i)}(r, t) A^{(s)}(r, t)$. The LSCS in a metal can be expressed in terms of the Fourier transforms of the field U and correlation function $\langle \langle \mathcal{N}(r, t) \mathcal{N}(r', t') \rangle \rangle$ with respect to $s - s', t - t', s = (x, y)$. In order to find the Fourier transform of the correlation function, we apply the general fluctuation-dissipation theorem [1-3] and express it by imaginary part of the susceptibility. Therefore, our problem is to find the susceptibility of the electron-phonon system in the external field $U(r, t)$.

2. Susceptibility and Fano resonance

After substitution of the screened vertex functions the Coulomb interaction can be disregarded up to frequencies $\omega \ll \omega_p$, and Boltzmann's equation is used in the τ -approximation.

The solution of Boltzmann's equation for the electron distribution function and the equation of motion for the phonon displacements with appropriate boundary conditions leads to

$$\begin{aligned} \chi(k_s, k_z, k'_z, \omega) &= 2\pi \delta(k_z - k'_z) \chi^{(b)}(k, \omega) - g_i(k_s, k_z, \omega) D_{i\alpha}^{(b)}(k_s, k_z, \omega) k_\alpha \\ &\quad \times D_{\alpha j}^{(s)}(k_s, \omega) \mu_{jzlm} D_{lk}^{(b)}(k_s, k'_z, \omega) g_k(k_s, k'_z, \omega) k'_m, \end{aligned} \quad (2)$$

where the contribution of acoustic phonons is omitted and

$$\chi^{(b)}(k, \omega) = \langle \gamma^2(p) \Pi(v \cdot k, \omega) \rangle + g_i(k, \omega) g_k(k, \omega) D_{ik}^{(b)}(k, \omega), \quad (3)$$

$$\Pi(v \cdot k, \omega) = \frac{i\tau^{-1} - v \cdot k}{\omega - v \cdot k + i\tau^{-1}}, \quad (4)$$

$$g_\alpha(k, \omega) = g_\alpha^{opt} - \langle \xi_\alpha(p) \gamma(p) \Pi(v \cdot k, \omega) \rangle. \quad (5)$$

The first term on the right hand side of (2) has the form typical of infinite space. It represents contributions (3) of the electron-hole pairs and bulk phonons. The poles of the matrix $D_{ik}^{(b)}(\mathbf{k}, \omega)$ determine the spectrum of the bulk optical phonons $\omega = \omega(\mathbf{k}) - i\Gamma(\mathbf{k}, \omega)$ with their damping (see Eq. (33) in [3]).

The second term in (2) represents an influence of the surface, the tensor μ results from the boundary conditions. The poles of matrix $D_{\alpha k}^{(s)}(\mathbf{k}_s, \omega)$ determine the spectrum of the surface optical phonons [3].

The LSCS in terms of the susceptibility has the form

$$\frac{d\sigma^{(b)}}{d\omega^{(s)}d\Omega^{(s)}} \propto \text{Im} \int \frac{dk_z}{2\pi} |U(\mathbf{k}, \omega)|^2 \chi^{(b)}(\mathbf{k}, \omega). \quad (6)$$

The influence of the surface is represented in (6) only by the integrand $|U(\mathbf{k}, \omega)|^2$ describing the distribution of the incident and scattered light. The imaginary part of the susceptibility for $k\nu \ll |\omega + i\tau^{-1}|$ has the following form:

$$\text{Im}\chi^{(b)}(\mathbf{k} = 0, \omega) = \langle \gamma^2(\mathbf{p}) \rangle \left[\frac{\omega\tau}{1 + \omega^2\tau^2} + \frac{(\tilde{g}_1^2 - \tilde{g}_2^2)\omega\Gamma_2 + \tilde{g}_1\tilde{g}_2(\tilde{\omega}^2 - \omega^2)}{(\tilde{\omega}^2 - \omega^2)^2 + 4\omega^2\Gamma_2^2} \right], \quad (7)$$

where $\tilde{\omega} = \omega(\mathbf{k}_s, k_z = \zeta_1)$, $\zeta_1 = \text{Re}\zeta$, $\Gamma_2 = \Gamma_2^{(i)} + \Gamma_2^{(e)}$,

$$\Gamma_2^{(e)} = \frac{\tau}{2\rho} \frac{\langle \xi^2(\mathbf{p}) \rangle}{1 + \omega^2\tau^2}, \quad \tilde{g}_1 = \frac{\tilde{g}}{\omega\tau} + g^{\text{opt}} \left(\frac{2}{\rho\langle \gamma^2(\mathbf{p}) \rangle} \right)^{\frac{1}{2}}, \quad (8)$$

$$\tilde{g}_2 = -\langle \xi(\mathbf{p})\gamma(\mathbf{p}) \rangle \left(\frac{2}{\rho\langle \gamma^2(\mathbf{p}) \rangle} \right)^{\frac{1}{2}} \frac{\omega\tau}{1 + \omega^2\tau^2}. \quad (9)$$

Here ζ is the sum of the normal components of the wave vector of the incident and scattered light in the metal. Using Eq. (7) we fit (see Fig. 1) the shape of the YBaCuO resonance line [4] with $\tilde{\omega} = 340 \text{ cm}^{-1}$ by the following parameters: $2\langle \xi(\mathbf{p})\gamma(\mathbf{p}) \rangle^2 / \rho\langle \gamma^2(\mathbf{p}) \rangle = 8100 \text{ cm}^{-2}$, $g^{\text{opt}} / \langle \xi(\mathbf{p})\gamma(\mathbf{p}) \rangle = -0.62$, $\tau^{-1} = 1030 \text{ cm}^{-1}$, $\Gamma_2(k = 0, \tilde{\omega}) = 9.9 \text{ cm}^{-1}$. The intrinsic phonon line width $\Gamma_2^{(i)} = 2.5 \text{ cm}^{-1}$ stems from a fit to the phonon line shape in the insulating state.

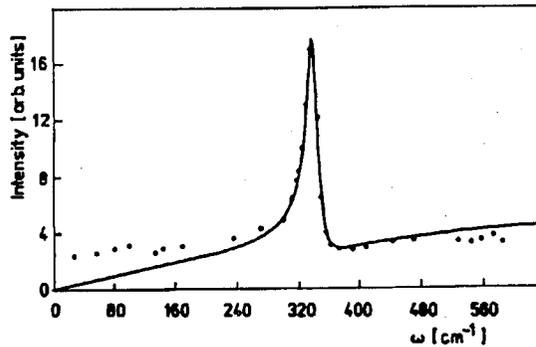


Fig. 1. Fit of Eq. (7) to 340 cm^{-1} resonance line of YBaCuO. The parameters used to get the fit are given in the text.

Our Eq. (7) contains the total phonon line width only. Therefore, this is essentially different from the formula (32) in Ref. [5] derived by the Green functions method, and including the total phonon line width and, in addition, an intermixture of the intrinsic phonon line width.

At low ω our results show deviation from experimental data shown in Fig. 1. The LSCS (6) vanishes if the frequency transfer ω goes to zero because the electron response is proportional to ω and the phonon damping Γ_2 is multiplied by ω . The last assumption was confirmed only for electron-phonon contribution $\Gamma_2^{(e)}$, but it seems natural that the intrinsic damping disappears also in static circumstances. In any case, if $\tilde{\omega}\Gamma_2$ appears in (7) instead of $\omega\Gamma_2$ we get at $\omega = 0$ a value $\text{Im}\chi(\omega = 0) = 4\tau\Gamma_2\text{Im}\chi(\tilde{\omega}) \approx 0.04\text{Im}\chi(\tilde{\omega})$, i.e. unmeasurable small value.

3. Summary

We evaluate the inelastic LSCS as the semiclassical response of a half-infinite metal. There are three contributions to the LSCS:

(i) the background is associated with excitation of the electron-hole pairs and is observed in the frequency transfer range $\omega \approx \max(v|\zeta|, \tau^{-1})$, where τ^{-1} is the temperature dependent collision rate for the electrons;

(ii) the light scattering may involve the excitation of a bulk phonon;

(iii) the excitation of surface optic phonons, which are similar to Rayleigh's waves, is possible. The longitudinal optical phonon slipping along the surface gives a nonsymmetrical peak.

One of us (L.A.F.) acknowledges the financial support by the Russian Foundation for Basic Research (grant No. 94-02-03029).

References

- [1] L.A. Falkovsky, S. Klama, *Phys. Rev. B* **50**, 5666 (1994).
- [2] L.A. Falkovsky, E.G. Mishchenko, *Phys. Rev. B* **51**, 7239 (1995).
- [3] L.A. Falkovsky, S. Klama, *Physica C* **264**, 1 (1996).
- [4] T. Staufer, R. Hackl, P. Müller, *Solid State Commun.* **75**, 975 (1991).
- [5] T.P. Devereaux, A. Virosztek, A. Zawadowski, *Phys. Rev. B* **51**, 505 (1995).