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Schwinger–Keldysh canonical formalism for electronic Raman scattering

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ABSTRACT

Inelastic low-energy Raman and high-energy X-ray scatterings have made great progress in instrumentation to investigate the strong electronic correlations in matter. However, theoretical study of the relevant scattering spectrum is still a challenge. In this paper, we present a Schwinger–Keldysh canonical perturbation formalism for the electronic Raman scattering, where all the resonant, non-resonant and mixed responses are considered uniformly. We show how to use this formalism to evaluate the cross section of the electronic Raman scattering off an one-band superconductor. All the two-photon scattering processes from electrons, the non-resonant charge density response, the elastic Rayleigh scattering, the fluorescence, the intrinsic energy-shift Raman scattering and the mixed response, are included. In the mean-field superconducting state, Cooper pairs contribute only to the non-resonant response. All the other responses are dominated by the single-particle excitations and are strongly suppressed due to the opening of the superconducting gap. Our formalism for the electronic Raman scattering can be easily extended to study the high-energy resonant inelastic X-ray scattering.

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1. Introduction

Inelastic low-energy Raman and high-energy X-ray scatterings have become powerful tools to study the strong electronic correlations in matter [1–3]. While the instrumental technique of the light scattering is in rapid progress, the theoretical study of the scattering spectrum is in less development. Two main difficulties suppress the theoretical study of the light scattering off the strongly correlated electrons. The first difficulty stems from the complexity of the strongly correlated electrons themselves. We now have no well-defined theoretical formalism for the various electronic correlations in such as the high-Tc cuprates, iron-based superconductors and heavy fermions, where the multiple comparable energy scales and different degrees of freedom are strongly correlated. The other difficulty lies in the description of the inelastic light scattering processes. Unlike the single-particle scattering technique such as the angle-resolved photoemission spectroscopy (ARPES) and neutron scattering, Raman and X-ray scatterings involve two-step photon-in photon-out processes. The cross section of the ARPES or neutron scattering is determined by the scattering correlation function which can be studied in perturbation formalism by the fluctuation–dissipation theorem. However, a simple extension of this formalism for the two-photon scattering is fail because the fluctuation–dissipation theorem is now invalid. We thus have no reliable perturbation formalism to study the scattering correlation function in Raman and X-ray scatterings.

In this paper, we focus our study on the second difficulty. We show that it can be overcome by introducing the Schwinger–Keldysh contour time formalism, which has been well established for non-equilibrium physics [4–6]. In this paper, we present a Schwinger–Keldysh perturbation formalism to evaluate the cross section of the electronic Raman scattering. The formalism for the high-energy resonant inelastic X-ray scattering (RIXS) can be established in a similar procedure.

Our starting point is the differential cross section of the inelastic light scattering. Consider a two-step photon-in photon-out scattering as shown schematically in Fig. 1. The incident photon with momentum $\mathbf{p}_i$ and polarization $\mathbf{e}_i$ is absorbed by the electrons of the target matter which then emits photon with momentum $\mathbf{p}_f$ and polarization $\mathbf{e}_f$. Suppose the initial state of the electrons is $|\phi_i\rangle$ at time t_i and the final state after the scattering is $|\phi_f\rangle$ at time t_f. The scattering probability of this two-photon process is described by

$$\Gamma(\mathbf{p}_f\mathbf{e}_f;\,\mathbf{p}_i\mathbf{e}_i) = \sum_{\phi_i\phi_f}\frac{1}{Z}e^{-\beta E_i}\left|\langle\Psi_F|\hat{S}(t_f,\,t_i)|\Psi_I\rangle\right|^2, \tag{1}$$

where $\hat{S}(t_f,\,t_i)$ is the time evolution matrix from an initial state $|\Psi_I\rangle \equiv |\mathbf{p}_i\mathbf{e}_i\phi_i\rangle$ into a final state $|\Psi_F\rangle \equiv |\mathbf{p}_f\mathbf{e}_f\phi_f\rangle$, and E_i is the energy of

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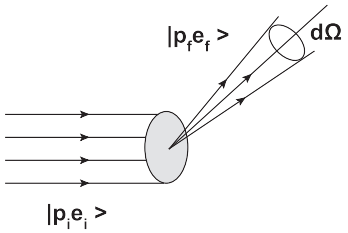

Fig. 1. Schematic light scattering from a target matter. $|\mathbf{p}_i\mathbf{e}_i\rangle$ and $|\mathbf{p}_f\mathbf{e}_f\rangle$ denote the incoming photon state with momentum $\mathbf{p}_i$ and polarization $\mathbf{e}_i$ and the scattered photon state with momentum $\mathbf{p}_f$ and polarization $\mathbf{e}_f$, respectively.

the electrons in the initial state. Suppose there are N photons in the initial state $|\mathbf{p}_i\mathbf{e}_i\rangle$. Among the N photons there are $N\sum_{\mathbf{p}_f\mathbf{e}_f} \Gamma(\mathbf{p}_f\mathbf{e}_f;\ \mathbf{p}_i\mathbf{e}_i)$ photons scattered. The conservation of the photons in the scattering process shows that

$$\Phi_i(\mathbf{p}_i,\ \mathbf{e}_i)\sigma\Delta t = N\sum_{\mathbf{p}_f\mathbf{e}_f} \Gamma(\mathbf{p}_f\mathbf{e}_f;\ \mathbf{p}_i\mathbf{e}_i), \tag{2}$$

where σ is the effective scattering cross section, $\Phi_i(\mathbf{p}_i,\ \mathbf{e}_i) = nc = Nc/V$ is the current density (or flux) of the incident photons (V is volume of the photon field and c is the light velocity), and $\Delta t = t_f - t_i$. Since $\omega_f = p_f c$, we have $\sum_{\mathbf{p}_f} = V/(2\pi c)^3 \int \omega_f^2\, d\omega_f\, d\Omega$ where $d\Omega$ is the differential solid angle. The double differential cross section with the initial and final photon states $|\mathbf{p}_i\mathbf{e}_i\rangle$ and $|\mathbf{p}_f\mathbf{e}_f\rangle$ is given by

$$\left.\frac{d^2\sigma}{d\Omega\, d\omega_f}\right|_{\mathbf{q},\nu} = \frac{V^2\omega_f^2}{(2\pi)^3c^4\Delta t}\Gamma(\mathbf{p}_f\mathbf{e}_f;\ \mathbf{p}_i\mathbf{e}_i), \tag{3}$$

where $\mathbf{q}$ and ν are the transferred momentum and energy frequency, respectively, and are defined by

$$\mathbf{q} = \mathbf{p}_i - \mathbf{p}_f, \quad \nu = \omega_i - \omega_f. \tag{4}$$

Formula (3) shows that the differential cross section is proportional to the scattering probability Γ. The time difference Δt can be canceled by an additional factor Δt in Γ which comes from the energy conservation law. Therefore $\Gamma/\Delta t$ can be taken as a scattering rate.

Suppose the coupling of the electron and the photon field is V_I. Define the total Hamiltonian of the combined system as $\mathcal{H} = H + H_p + V_I$ with H and H_p being the Hamiltonian of the electron and the photon system respectively, $\hat{S}$ matrix is given by

$$\hat{S}(t_f,\ t_i) = T_t e^{-i/\hbar\int_{t_i}^{t_f} dt V_I(t)}, \tag{5}$$

where $V_I(t) = e^{i/\hbar(H+H_p)(t-t_i)}V_I e^{-i/\hbar(H+H_p)(t-t_i)}$ and T_t is the time ordering operator. Separate the interaction V_I into V_1 of linear to $\mathbf{A}$ and V_2 of quadratic to $\mathbf{A}$, where $\mathbf{A}$ is the photon vector potential. To lowest-order perturbations, only the following two expansions of the $\hat{S}$ matrix contribute to the scattering probability Γ,

$$\Gamma = \sum_{\phi_i\phi_f}\frac{e^{-\beta E_i}}{Z}\left|\langle\Psi_F|\hat{S}_1 + \hat{S}_2|\Psi_I\rangle\right|^2, \tag{6}$$

where $\hat{S}_{1,2}$ are defined by

$$\hat{S}_1 = -\frac{i}{\hbar}\int_{t_i}^{t_f} dt V_2(t),$$
$$\hat{S}_2 = \frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2\int_{t_i}^{t_f} dt_1\, dt_2 T_t\left[V_1(t_1)V_1(t_2)\right]. \tag{7}$$

Thus the scattering probability Γ involves three contributions,

$$\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_{12}, \tag{8}$$

with

$$\Gamma_1 = \sum_{\phi_i\phi_f}\frac{e^{-\beta E_i}}{Z}\left|\langle\Psi_F|\hat{S}_1|\Psi_I\rangle\right|^2,$$
$$\Gamma_2 = \sum_{\phi_i\phi_f}\frac{e^{-\beta E_i}}{Z}\left|\langle\Psi_F|\hat{S}_2|\Psi_I\rangle\right|^2,$$
$$\Gamma_{12} = \sum_{\phi_i\phi_f}\frac{e^{-\beta E_i}}{Z}2\,\mathrm{Re}\left[\langle\Psi_I|\hat{S}_1^{\dagger}|\Psi_F\rangle\langle\Psi_F|\hat{S}_2|\Psi_I\rangle\right]. \tag{9}$$

Γ_1, Γ_2 and Γ_{12} are the so-called *non-resonant*, *resonant* and *mixed* parts of the scattering probability, respectively. Γ_{12} describes quantum interference of the resonant and non-resonant scattering processes. The positive or negative Γ_{12} comes from the corresponding constructive or destructive quantum interference.

Since the states of the incident and the scattered photons are defined definitely, the scattering probability Γ can be reduced into a representation of the pure electron system. Now $\hat{S}_{1,2}$ matrices can be re-expressed in similar forms to Eq. (7) where the interactions $V_{1,2}$ are substituted by the reduced ones $\mathcal{V}_{1,2}$ without photon field involved (details and derivation will be shown in the following section).

The non-resonant scattering probability Γ_1 is determined by the correlation function as

$$\Gamma_1 = \int_{t_i}^{t_f} dt_1 dt_2\langle\mathcal{V}_2^{\dagger}(t_1)\mathcal{V}_2(t_2)\rangle, \tag{10}$$

where $\langle\hat{A}\rangle \equiv 1/Z\,\mathrm{Tr}[e^{-\beta H}\hat{A}]$ and $\mathcal{V}(t) = e^{i/\hbar H(t-t_i)}\mathcal{V}e^{-i/\hbar H(t-t_i)}$. With the fluctuation–dissipation theorem, Γ_1 can be re-expressed into the standard form:

$$\Gamma_1 = \frac{2\Delta t}{1-e^{-\beta\nu}}\,\mathrm{Im}\,\chi(\nu), \tag{11}$$

where $\chi(\nu)$ is the frequency Fourier transformation of the time-ordered correlation function $\chi(t_1,\ t_2) = i\theta(t_1 - t_2)\langle[\mathcal{V}_2^{\dagger}(t_1),\ \mathcal{V}_2(t_2)]\rangle$. Perturbation theory can then be easily introduced to evaluate Γ_1. This is a standard formalism to study the scattering probability in the single-particle scattering technique such as ARPES and neutron scattering.

Because of the time ordering operator $T_t[\mathcal{V}_1(t_1)\mathcal{V}_1(t_2)]$ in $\hat{S}_2$ matrix, the fluctuation–dissipation theorem is invalid to evaluate the resonant Γ_2 and the mixed Γ_{12}. In most studies of the Raman or the X-ray scattering spectrum, Γ_2 and Γ_{12} are evaluated from the Kramers–Heisenberg formula [1,3], where the perturbation is badly controlled and numerical methods are applied. No reliable perturbation formalism is established even for the weakly interacting electron system. The time ordering in $\hat{S}_2$ matrix is the difficulty we should overcome to establish a perturbation formalism to evaluate Γ_2 and Γ_{12}.

From the picture of a time evolution, the scattering probability Γ involves two time evolution processes, forward time ordering from the initial state $|\Psi_I\rangle$ at t_i to the final state $|\Psi_F\rangle$ at t_f, and backward anti-time ordering from the final state $|\Psi_F\rangle$ back to the initial state $|\Psi_I\rangle$. Introducing an anti-time ordering evolution matrix $\tilde{S}$,

$$\tilde{S}(t_i,\ t_f) = \tilde{T}_t e^{-i/\hbar\int_{t_f}^{t_i} dt V_I(t)}, \tag{12}$$

we can then define the anti-time ordering $\tilde{S}_{1,2}$ matrices analog to $\hat{S}_{1,2}$ in Eq. (7). Following the time-and-anti-time evolution picture, Γ_2 can be expressed as

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