Electronic Raman Dynamical Structure Factor

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The non-perturbative Hamiltonian is H_0, and the effective perturbative Hamiltonian H' is

$$\begin{aligned} H' &= -e\frac{4\pi n(\vec{q},\omega)}{q^2}e^{-i\omega t}\sum_{\vec{k},\sigma}\gamma_{\vec{k}}c^\dagger_{\vec{k}+\vec{q}\sigma}c_{\vec{p}\sigma} \\ &= -e\phi(\vec{q},\omega)e^{-i\omega t}\tilde{\rho}^\dagger_{\vec{q}} \end{aligned} \tag{1}$$

where $\phi(\vec{q},\omega) = \dfrac{4\pi n_t(\vec{q},\omega)}{q^2}$ represents the potential induced by the charge $n(\vec{q},\omega)$.

When the total Hamiltonian is $H = H_0 + H'$, the following difference is obtained by electronic Raman scattering experiments: $\Delta\tilde{\rho}_{\vec{q}} = \langle\tilde{\rho}_{\vec{q}}\rangle_H - \langle\tilde{\rho}_{\vec{q}}\rangle_{H_0}$

This is expressed using the external force $F(t) = e\phi(\vec{q},\omega)e^{-i\omega t}$:

$$\Delta\tilde{\rho}_{\vec{q}} = -\int_{-\infty}^{t} dt' F(t')\chi^{(R)}_{\tilde{\rho}\tilde{\rho}}(t-t') \tag{2}$$

Here $\chi^{(R)}_{\tilde{\rho}\tilde{\rho}}$, which is often called the response function (of the retarded part), was shown by R. Kubo in the linear response regime and is known as the Kubo formula.

$$\chi^{(R)}_{\tilde{\rho}\tilde{\rho}}(t) = -i\theta(t)\big\langle[\tilde{\rho}_{\vec{q}}(t),\tilde{\rho}^\dagger_{\vec{q}}]\big\rangle \tag{3}$$

where the thermal average $\langle\cdots\rangle$ can be expanded by using the thermodynamic potential Ω and orthonormal vectors $\big\{|n\rangle\big\}$ which satisfy $H|n\rangle = E_n|n\rangle$

$$\begin{aligned} \big\langle[\tilde{\rho}_{\vec{q}}(t),\tilde{\rho}^\dagger_{\vec{q}}]\big\rangle &= \mathrm{Tr}\Big[e^{\beta(\Omega-H)}\big(e^{iHt}\tilde{\rho}_{\vec{q}}e^{-iHt}\tilde{\rho}^\dagger_{\vec{q}} - \tilde{\rho}^\dagger_{\vec{q}}e^{iHt}\tilde{\rho}_{\vec{q}}e^{-iHt}\big)\Big] \\ &= e^{\beta\Omega}\sum_{m,n}e^{i(\beta E_n - E_m)t}\big|\langle n|\tilde{\rho}_{\vec{q}}|m\rangle\big|^2\Big(e^{-\beta E_n} - e^{-\beta E_m}\Big) \end{aligned} \tag{4}$$

After Fourier transformed, it can be also written as

$$\chi^{(R)}_{\tilde{\rho}\tilde{\rho}}(\vec{q},\omega) = -i\int_0^\infty dt\ \big\langle[\tilde{\rho}_{\vec{q}}(t),\tilde{\rho}^\dagger_{\vec{q}}]\big\rangle \tag{5}$$

Generally, the scattering probability is proportional to the dynamical structure factor in the Born approximation.

$$S(\vec{q},\omega) = e^{\beta\Omega}\sum_{m,n}e^{-\beta E_n}\big|\langle n|\rho_{\vec{q}}|m\rangle\big|^2\delta(E_n - E_m + \omega) \tag{6}$$

From the correspondence between $\chi^{(R)}_{\tilde{\rho}\tilde{\rho}}$ and the dynamical structure factor, we should define the electronic Raman dynamical structure factor $\tilde{S}(\vec{q},\omega)$ as follows.

$$\begin{aligned} \tilde{S}(\vec{q},\omega) &= e^{\beta\Omega}\sum_{m,n}e^{-\beta E_n}\big|\langle n|\tilde{\rho}_{\vec{q}}|m\rangle\big|^2\delta(E_n - E_m + \omega) \\ &= -\frac{1+\coth(\beta\omega/2)}{2\pi}\mathrm{Im}\chi^{(R)}_{\tilde{\rho}\tilde{\rho}}(\vec{q},\omega) \end{aligned} \tag{7}$$