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**A True Meaning of Frequency Dependent Elastic Constants**

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A physical origin of frequency dependences in elastic constants, which are often found in ultrasound propagation in filled-skutterudites and clathrate compounds[1, 2, 3], is investigated. We use the following Hamiltonian including interactions between local phonons and lattice phonons (or conduction electrons):

$$H = \sum_{\alpha \mathbf{i}} E_\alpha \phi^\dagger_{\mathbf{i}\alpha}\phi_{\mathbf{i}\alpha} + H_{\rm ph} + H_{\rm hyb}, \tag{1}$$

$$H_{\rm ph} = \sum_{n\mathbf{k}} \omega_{\mathbf{k}n} b^\dagger_{n\mathbf{k}} b_{n\mathbf{k}}, \qquad H_{\rm hyb} = \frac{1}{\sqrt{N_0}} \sum_{n\mathbf{k}\mathbf{i}\alpha\beta} e^{\imath \mathbf{k}\mathbf{x}_\mathbf{i}} v^{\alpha\beta}_{n\mathbf{k}} \phi^\dagger_{\mathbf{i}\alpha}\phi_{\mathbf{i}\beta}(b^\dagger_{n-\mathbf{k}} + b_{n\mathbf{k}}). \tag{2}$$

Here $\phi^\dagger_\alpha$ is the auxiliary Fermionic operator that creates the local phonon with the energy $E_\alpha$. $b^\dagger_{n\mathbf{k}}$ is the creation operator of the lattice phonon with the wave number $\mathbf{k}$ and the symmetry index $n$. $N_0$ is the number of the sites. The coefficient $v^{\alpha\beta}_{n\mathbf{k}}$ represents "hybridization" between the local and the lattice phonons. It is noted that $v^{\alpha\beta}_{n\mathbf{k}}$ is the Fourier transformation of the matrix element of the local displacement $(X^n_\mathbf{i})_{\alpha\beta}$ $(n = 1, 2, 3)$ in the lowest order in $X^n_\mathbf{i}$. This Hamiltonian can be seen as the bosonic version of Anderson lattice. In the case of a electron-phonon interaction, $H_{\rm ph} + H_{\rm hyb}$ should be replaced by

$$\sum_{nm\mathbf{k}\sigma} \epsilon^{nm}_\mathbf{k} c^\dagger_{n\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \frac{1}{\sqrt{N_0}} \sum_{n\mathbf{k}\mathbf{i}} \sum_{\alpha\beta\sigma} \gamma^n_\mathbf{k} (Q^n_\mathbf{i})_{\alpha\beta} \psi^\dagger_{\mathbf{i}\alpha}\psi_{\mathbf{i}\beta} e^{\imath \mathbf{k}\mathbf{x}_\mathbf{i}} n_{n\mathbf{k}\sigma}, \tag{3}$$

where $n_{n\mathbf{k}\sigma}$ is the density of the electron with the wave number $\mathbf{k}$, the spin $\sigma$, and the other index $n$. $c^\dagger_{n\mathbf{k}\sigma}$ is the creation operator of the conduction electrons with the energy $\epsilon^{nm}_\mathbf{k}$(including the off-diagonal elements). $Q^n_\mathbf{i}$ is written by the linear conbination of $X_\mathbf{i}$ and $\gamma^n_\mathbf{k}$ is coupling constants.

Using pseudoparticle methods, we evaluate the selfenergy of the local phonon and the elastic constants. The discussion is all based on a singlet ground state model for the local phonon system, that is demanded in this kind of non-magnetic one-body potential problem. From our results, we can see the frequency dependence arises from the excited degenerate states. It is also concluded that the relaxation time does not represent the height of the off-center potential hill for ions. The most importance is the existence of the dissipative environment coupled with the local phonon system. In filled-skutterudites case, this environment is thought to be d-electrons at the transition metal sites from the various experimental results. This expectation is confirmed by our analysis and its electron-local phonon interacting Hamiltonian is proposed (eq. (4)). We discuss the irrelevancy of the conduction electrons that arise from the $A_u$ molecular orbital of pnictogen cages. The results for simplified models will be discussed in the presentation.

# References

[1] T. Goto *et al.*: Phys. Rev. B **69** (2004) 180511(R).

[2] Y. Nemoto *et al.*: Phys. Rev. B **68** (2003) 184109.

[3] T. Goto *et al.*: Phys. Rev. B **70** (2004) 184126.