Memory Effects in the Energy Dissipation of Anharmonic Solids

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TRANSPORT IN SOLIDS OUT OF EQUILIBRIUM

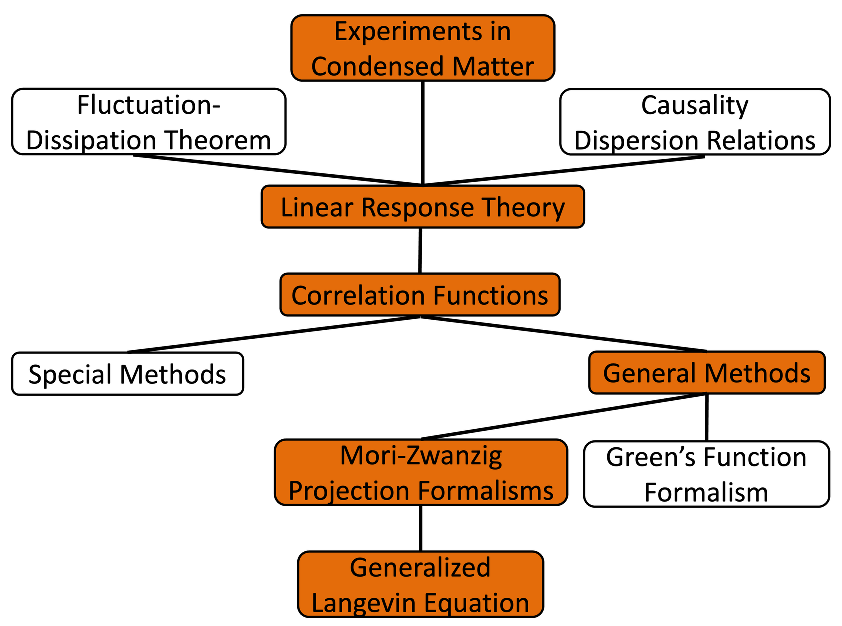

Figure 1. Experiment and theory stages in Condensed Matter Physics.

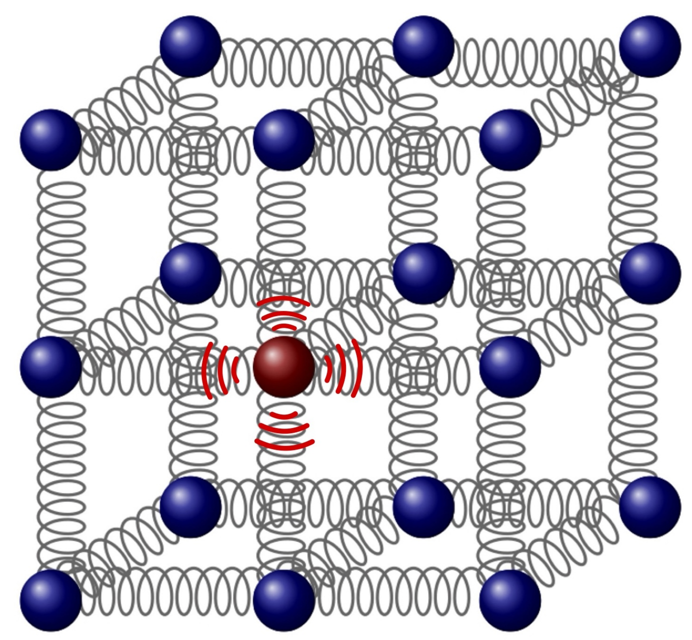

Figure 2. Pictorial representation of the vibrations in a solid given a local perturbation.

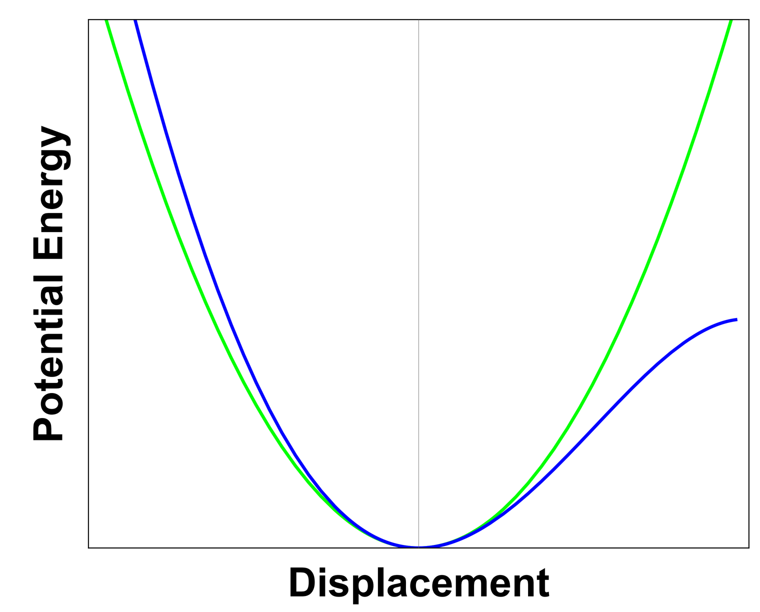

Figure 3. Interatomic potential energy comparison between a harmonic potential and an anharmonic potential of the type $U(r) = kr^2/2 - Jr^3 - Kr^4$.

Phonon Scattering and Energy Dissipation

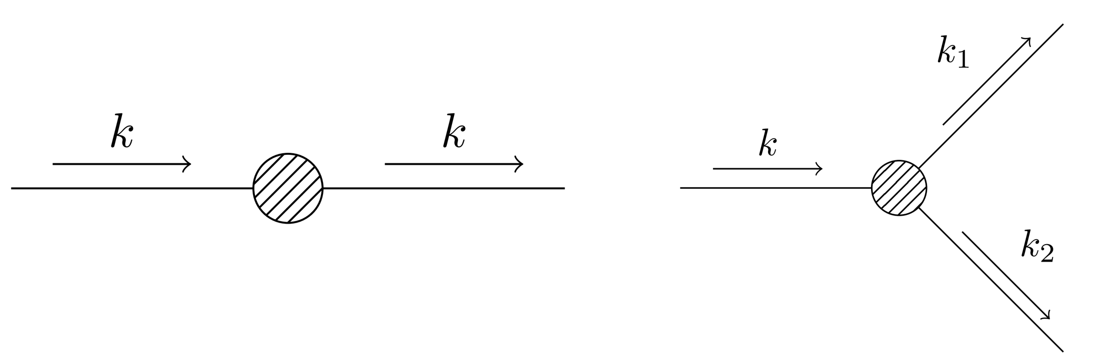

Figure 4. 2–phonon process (ballistic) and 3–phonon process (diffusive) diagrams.

Thermal Conductivity

General Definition	$\vec{J} = -\overset{\leftrightarrow}{\kappa} \cdot \vec{\nabla} T$
Linear Response (Green–Kubo)	$\kappa_{i,j} = \frac{1}{T}(\hat{J}_i(t), \hat{J}_j)$
Peierls Expression (1D)	$\hat{J}(t) = \sum_k (\partial_k \Omega_k)\Omega_k \hat{n}_k(t)$

Table 1. Relation between thermal conductivity κ and heat current density $\hat{J}$.

THEORETICAL FRAMEWORK

Time Evolution and Mori Projection [1]

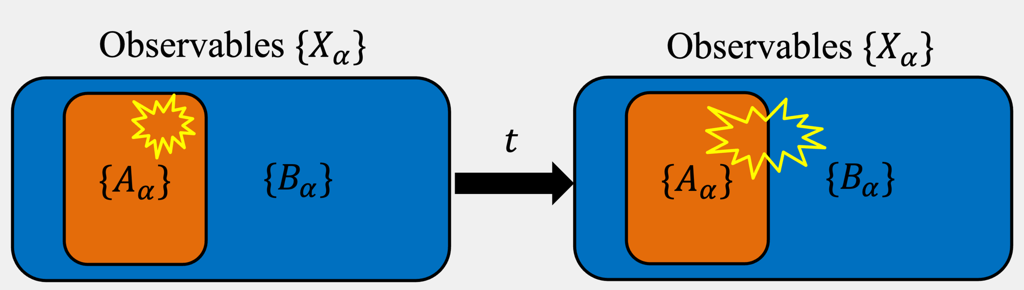

Figure 5. Time evolution of an operator in the active subspace.

Projector into active subspace

$$\mathcal{P}\bullet = \sum_\alpha \hat{A}_\alpha \left(\hat{A}_\alpha, \bullet\right) .$$

Anharmonic Quantum Oscillators [2]

Harmonic Hamiltonian

$$\mathcal{H}_H = \sum_k \left[\frac{\hat{P}_k^\dagger \hat{P}_k}{2m} + \frac{m\Omega_k^2}{2}\hat{Q}_k^\dagger \hat{Q}_k\right] ,$$

where Ω_k is the phonon frequency.

(Weak) Anharmonic Hamiltonian

$$\mathcal{H}_A = -\sum_{k_1,k_2,k_3} J(k_1,k_2,k_3)\hat{Q}_{k_1}\hat{Q}_{k_2}\hat{Q}_{k_3} - \sum_{k_1,k_2,k_3,k_4} K(k_1,k_2,k_3,k_4)\hat{Q}_{k_1}\hat{Q}_{k_2}\hat{Q}_{k_3}\hat{Q}_{k_4} .$$

where $J(k_1,k_2,k_3)$, $K(k_1,k_2,k_3,k_4)$ are coupling constants that include momenta conservation.

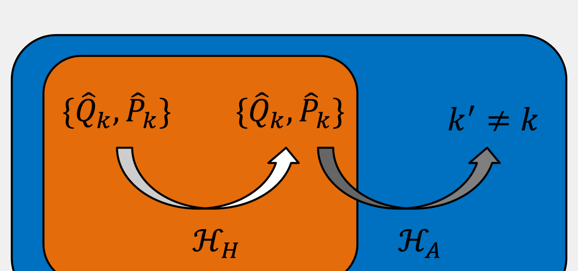

Figure 6. Time evolution of the variables with respect to the harmonic Hamiltonian $\mathcal{H}_H$ and anharmonic Hamiltonian $\mathcal{H}_A$.

Generalized Langevin Equation [2, 1]

$$\partial_t \hat{A}_\alpha(t) = \sum_\beta \underbrace{i\Omega_{\alpha,\beta}}_{\text{frequency matrix}} \hat{A}_\beta(t) - \sum_\beta \int_0^t \mathrm{d}t' \underbrace{M_{\alpha,\beta}(t-t')}_{\text{memory function}} \hat{A}_\beta(t') + \underbrace{\hat{f}_\alpha(t)}_{\text{random force}}$$

$$\partial_t \Phi_{\alpha,\beta}(t) = \sum_\gamma i\Omega_{\alpha,\gamma}\Phi_{\gamma,\beta}(t) - \sum_\gamma \int_0^t \mathrm{d}t' \underbrace{M_{\alpha,\gamma}(t-t')}_{\text{non-linear effects}} \Phi_{\gamma,\beta}(t') ,$$

where $\Phi_{\alpha,\beta}(t) = \left(\hat{A}_\alpha, \hat{A}_\beta(t)\right)$ are the relaxation functions and $(\bullet, \bullet)$ denotes the Kubo–Mori–Bogoliubov inner product [3].

Displacement Relaxation Function [2]

$$\widetilde{R}_k(z) = \int_0^\infty \mathrm{d}t\, e^{izt} \frac{\left(\hat{Q}_k, \hat{Q}_k(t)\right)}{\left(\hat{Q}_k, \hat{Q}_k\right)} = \frac{-iz + \widetilde{M}_k(z)}{-iz\left(-iz + \widetilde{M}_k(z)\right) + \chi_k^{-1}} .$$

Memory Function

$$\widetilde{M}_k(z) \approx -iz\frac{9}{m^3}\sum_{p,q}\frac{|J(-k,p,q)|^2}{\Omega_p\Omega_q}\left[\frac{1}{\Omega_+}\frac{1+n_q+n_p}{\Omega_+^2 - z^2} + \frac{1}{\Omega_-}\frac{n_q - n_p}{\Omega_-^2 - z^2}\right] ,$$

with $\Omega_\pm = \Omega_p \pm \Omega_q$, the emission/absorption frequencies, and $n_k = (1 - e^{-\beta\hbar\Omega_k})^{-1}$ the occupation number. This quantity can be related with the self–energy (Green's function formalism) through the relation: $\Sigma_k(t) = \partial_t M_k(t)$.

Static Susceptibility

$$\chi_k^{-1} = \frac{m\beta}{\left(\hat{Q}_k, \hat{Q}_k\right)} \approx \Omega_k(T)^2 - M_k(t=0) .$$

Here, $\Omega_k(T)$ corresponds to the corrected phonon frequency including the corrections from the quartic interaction.

LINEAR ANHARMONIC CHAIN

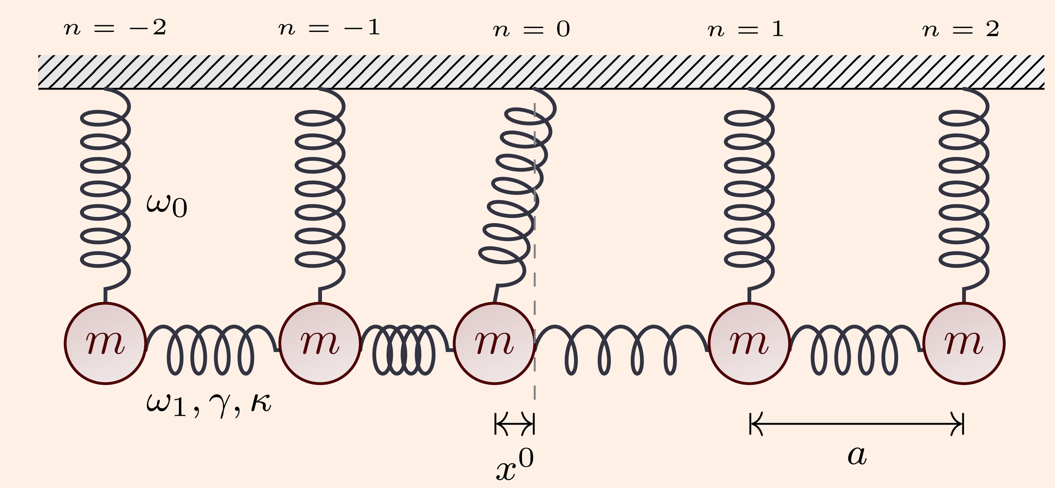

Figure 7. Pictorial representation of the model in the real space in 1D.

Relaxation due to an Adiabatic External Force [4]

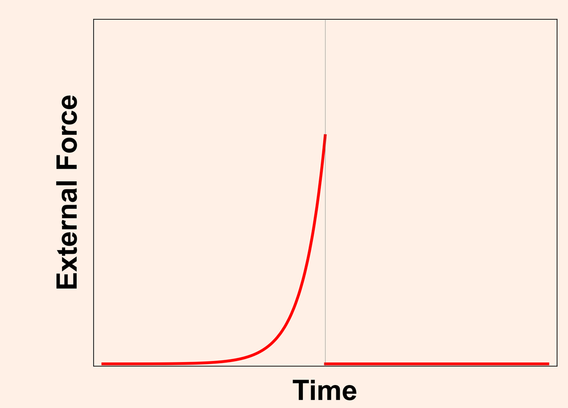

Figure 8. Adiabatic external force plot; $\mathcal{H}_{ext}(t) = -\sum_k \hat{Q}_k^\dagger F_k e^{\epsilon t}\theta(-t)$, $\epsilon \to 0^+$.

Displacement

$$\delta\left\langle \hat{Q}_k(z)\right\rangle = \widetilde{R}_k(z)\underbrace{\delta\left\langle \hat{Q}_k(t=0)\right\rangle}_{=\frac{\chi_k F_k}{m}} .$$

If only the central mass is initially displaced, then

$$\delta\langle \hat{x}_n(t)\rangle = x_0\frac{1}{N}\sum_k e^{ikn}R_k(t) .$$

NUMERICAL RESULTS FOR DISPLACEMENT AND ENERGY DISSIPATION [1]

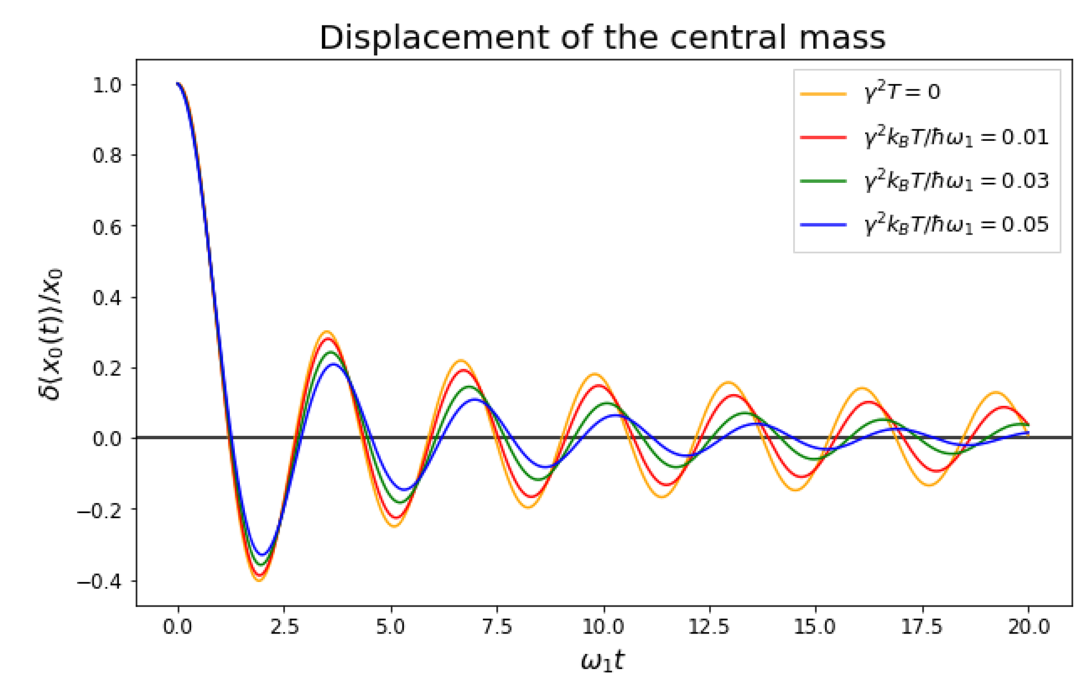

Figure 9. In the high temperature limit: Displacement of the central mass for different values of cubic anharmonicity coupling.

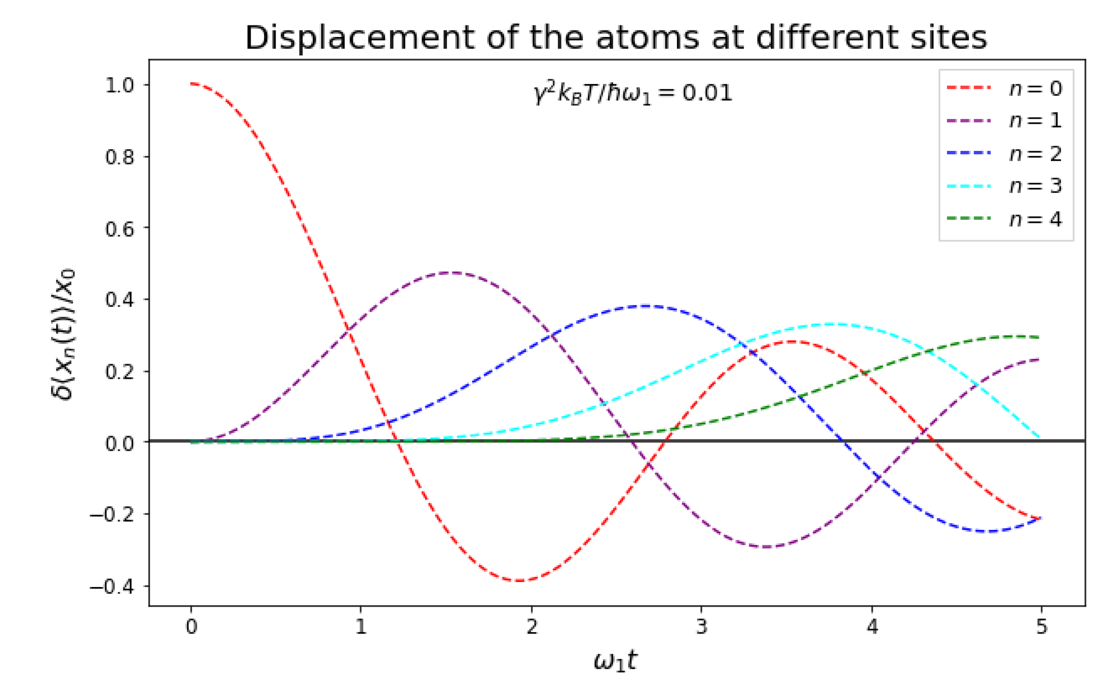

Figure 10. In the high temperature limit: Displacement of the atoms in different sites for $\gamma^2 k_B T/\hbar\omega_1 = 0.01$.

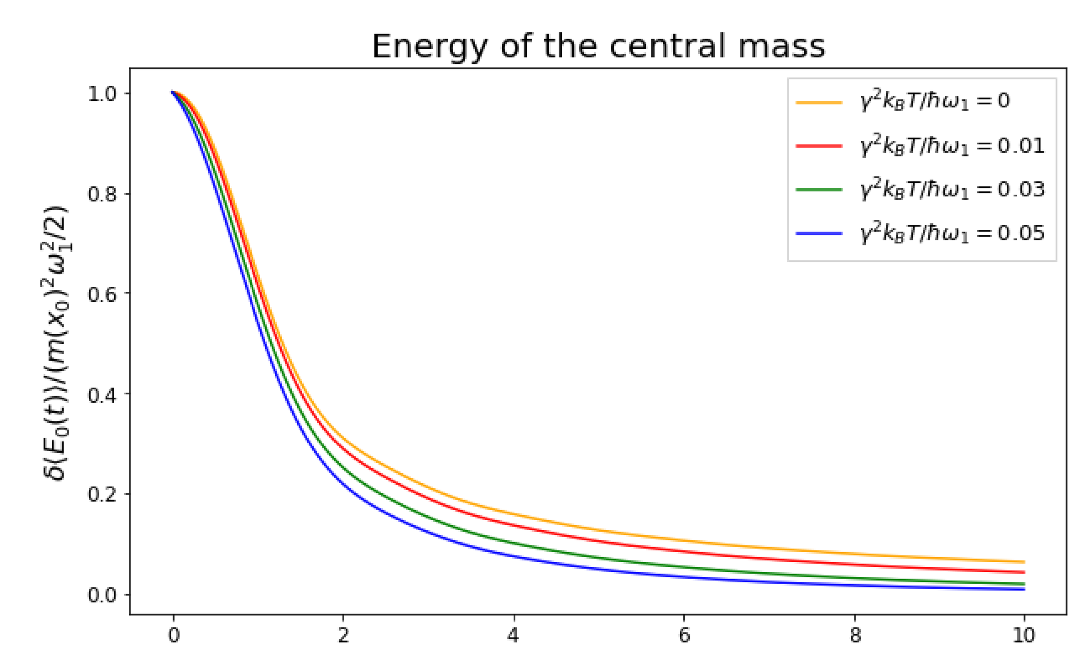

Figure 11. In the high temperature limit: Energy of the central mass for different values of cubic anharmonicity coupling using the decoupling approximation.

Note: γ corresponds to a dimensionless variable representing the constant cubic interatomic coefficient in the real space.

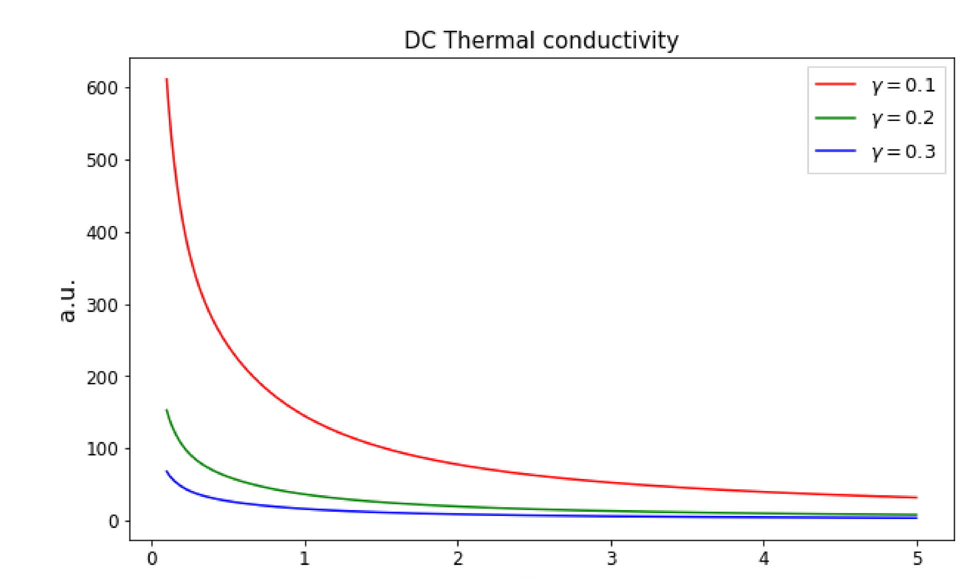

Figure 12. DC thermal conductivity of the 1D model via Peierls expression [5].

$$\kappa_{\mathrm{DC}} \approx \frac{1}{ak_B T^2}\frac{1}{N}\sum_k \frac{\Omega_k^2(\partial_k\Omega_k)^2\left(-n'(\epsilon_k)\right)}{2\Gamma_k} ,$$

with ϵ_k the perturbed energy and $\Gamma_k \equiv \mathrm{Re}[\widetilde{M}_k(\epsilon_k + i0^+)]$ the damping coefficient.

Conclusions

1. We were able to study analytically and numerically the dynamics of a system upon an external perturbation.
2. We determined the contribution of anharmonicites to the time evolution of dynamical variables of a simplified 1D model.

Future Work and Applications

1. Implement the dissipation effects of phonon scattering to compute the conductivity of a material in ab–initio codes beyond the relaxation–time approximation.
2. Application to quantum computing: reduction of quantum decoherence in qubits embedded in solid materials.

References

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[2] S. Lovesey, *Condensed matter physics: Dynamic correlations*. Benjamin/Cummings, 1986.

[3] R. Kubo, "The fluctuation-dissipation theorem," *Reports on Progress in Physics*, vol. 29, p. 255, jan 1966.

[4] D. Forster, T. C. Lubensky, P. C. Martin, J. Swift, and P. S. Pershan, "Hydrodynamics of liquid crystals," *Phys. Rev. Lett.*, vol. 26, pp. 1016–1019, 1971.

[5] B. Deo and S. N. Behera, "Calculation of thermal conductivity by the kubo formula," *Phys. Rev.*, vol. 141, pp. 738–741, Jan 1966.

[1] We took 10001 points in the to compute the k-sums. To compute the inverse Laplace transform, we related it with the Fourier transform, which needs to include a small imaginary parameter $i\eta$, we took $\eta = 0.001$. This introduces a small damping $e^{-\eta t}$, which was taken into account in the plots. We used 2000 points for $\omega \in [0, 2]$.