Study phonon transport by using Kubo method

Wu Li[1,2], **H. Sevinçli**[2], **S. Roche**[3,2] **and G. Cuniberti**[2]

[1]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

[2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

[3]Institute for Nanoscience and Cryogenics INAC/SP2M/L_Sim, CEA, 38054 Grenoble Cedex 9, France

We propose employing the real space Kubo method, which has already been well applied to the electronic transport, to study the phonon transport. As an application of this method, we calculated the phonon mean free path in an isotopic carbon nanotube system. The results are shown to be in good agreement with those obtained by using the GF approach, with the exception of low frequency modes, which is due to the limitation of computation time.

Kubo thermal conductance

•System Hamiltonian: $$\hat{\mathcal{H}} = \sum_i \frac{\hat{p}_i^2(t)}{2M_i} + \sum_{ij} \Phi_{ij}\hat{u}_i\hat{u}_j$$

•Phonon conductivity: $$\kappa = \frac{V}{T}\int_0^\beta d\lambda \int_0^\infty dt \langle \hat{J}^x(-i\hbar\lambda)\hat{J}^x(t)\rangle$$

energy flux operator

$$\hat{J}^x = \frac{1}{2V}\sum_{ij}(X_i - X_j)\Phi_{ij}\hat{u}_i\hat{v}_j$$

After some straightforward algebra

$$\kappa = \frac{\hbar^2\beta}{2\pi VT}\int_0^\infty d\omega \frac{-\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\mathrm{Tr}\{[X,D]\delta(\omega^2-D)[X,D]\delta(\omega^2-D)\}$$

•1D conductance $$\sigma = \frac{\hbar^2\beta}{2\pi L^2 T}\int_0^\infty d\omega \frac{-\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\mathrm{Tr}\{[X,D]\delta(\omega^2-D)[X,D]\delta(\omega^2-D)\}$$

Introducing Schrödinger kind of evolution operator

$$U(t) = e^{-i\hbar\beta Dt}$$

and rewrite the conductance in terms of transmission function

$$\sigma = \frac{\hbar^2\beta}{2\pi T}\int_0^\infty d\omega \frac{\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}T(\omega)$$

phonon $$T(\omega) = \frac{1}{L^2}\frac{1}{(\hbar\beta)^2}\mathrm{Tr}\{V_x\delta(\omega^2-D)V_x\delta(\omega^2-D)\}$$

electron $$T_{el}(E) = \frac{\hbar^2}{L^2}\mathrm{Tr}\{\hat{V}_x\delta(E-\hat{\mathcal{H}})\hat{V}_x\delta(E-\hat{\mathcal{H}})\}$$

in the same form

Numerical approach [1,2,3,4]

•Transmission function of a system of length L

$$T(E,L) = \frac{2\pi}{\hbar\beta L}\mathrm{Tr}[\delta(\omega^2-D)]\mathcal{D}(\omega,\tau_L)$$

diffusion coefficient — propagation time over L

$$\mathcal{D}(\omega,t) = \frac{\chi^2(\omega,t)}{t} = \frac{1}{t}\frac{\mathrm{Tr}\{[\hat{X}(t)-\hat{X}(0)]^2\delta(\omega^2-D)\}}{\mathrm{Tr}[\delta(\omega^2-D)]} = \frac{1}{t}\frac{\mathrm{Tr}\{[X,U(t)]^\dagger\delta(\omega^2-D)[X,U(t)]\}}{\mathrm{Tr}[\delta(\omega^2-D)]}$$

•The trace can be efficiently computed through an average over random phase states

$$\mathrm{Tr}[\delta(\omega^2-D)] \approx N \times \overline{\langle\psi|\delta(\omega^2-D)|\psi\rangle}$$

LDOS calculated by the continued fraction method

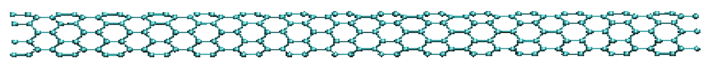
$$\mathrm{Tr}[X,U(t)]^\dagger\delta(\omega^2-D)[X,U(t)] \approx N \times \overline{\langle\psi|[X,U(t)]^\dagger\delta(\omega^2-D)[X,U(t)]|\psi\rangle}$$

computed by using Chebyshev expansion of U(t)

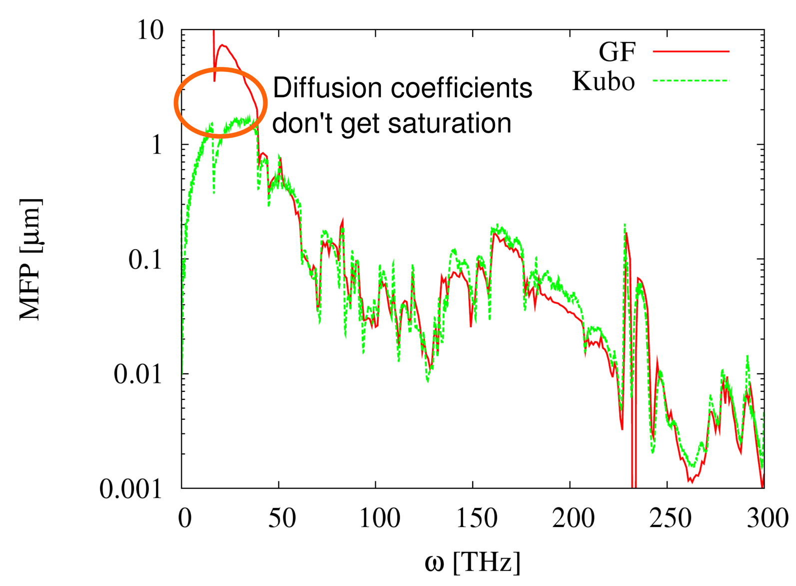
•Mean free path $$l(\omega) = \frac{\mathcal{D}_{max}(\omega)}{v(\omega)}$$

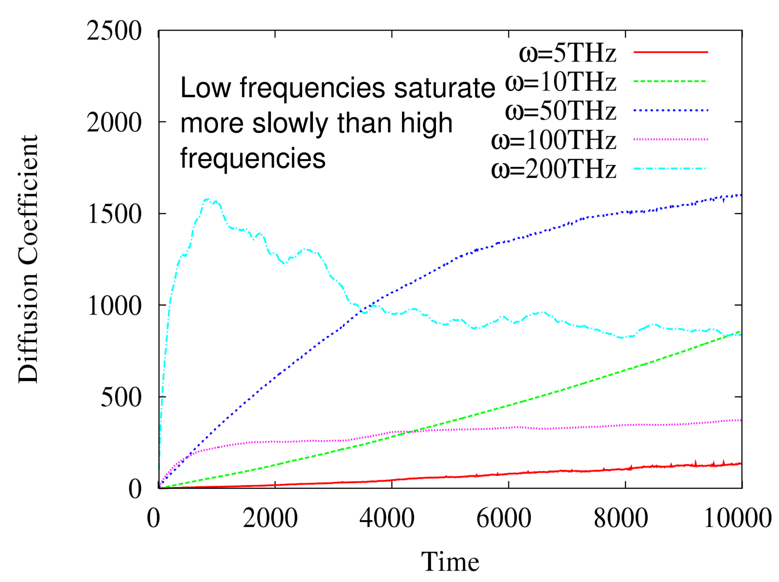
Results

Test Case: (7, 0) CNT with 10.7% of ^{14}C isotope



$l = 1.70\mu m$





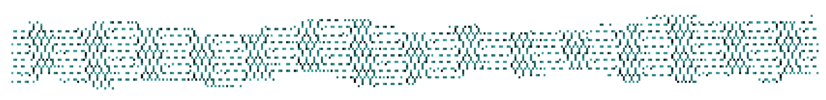
•Good agreement with GF result [5] at high frequencies
•Very efficient for high frequencies and large systems
•Difficult to get the MFP for low frequencies due to the limitation of computation time

Conclusion and Discussion

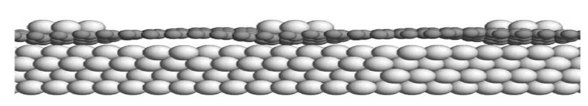
•By introducing a Schrödinger type of evolution operator, the phonon Kubo transmission function is found to be in the same form as the electronic transmission function
•The numerical Kubo method which is very efficient to treat the electronic transport can be applicable to phonon transport in principle
•For the isotopic disorder (7, 0) CNT, MFP down to the second conduction plateau can be obtained within acceptable computation time
•The thermal conductance is mainly contributed by the low frequency modes, and therefore it is more practical to apply this method to strongly disordered system of which the low frequency phonon modes are diffusive

•Work in progress

edge disordered GNRs



pinned graphene [6]



References

[1] S.Roche and D.Mayou, Phys. Rev. Lett **79**, 2518 (1997)
[2] S.Roche, Phys. Rev. B **59**, 2284 (1999)
[3] F.Triozon, J.Vidal, R.Mosseri and D.Mayou, Phys. Rev. B **65**, 220202(R) (2002)
[4] F.Triozon, S.Roche, A.Rubio and D.Mayou, Phys. Rev. B **69,** 121410(R) (2004)
[5] I.Savic, N.Mingo and D.Stewart, Phys. Rev. Lett **101**, 165502 (2008)
[6] P.J.Feibelman, Phys. Rev. B **77**, 165419 (2008)