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Influence of Thermal Fluctuations on the Conductance of Metallic Carbon Nanotubes

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Abstract: We study the influence of temperature-induced structural lattice fluctuations on the elastic electron transport in single-wall carbon nanotubes within a density-functional-based scheme. In the linear response regime, the linear conductance is calculated via configurational averages over the distorted lattice. Results obtained from a frozen-phonon approach as well as from molecular dynamics simulations are compared. We further demonstrate that the effect of structural fluctuations can be approximately captured by the Anderson model of disorder. The influence of individual vibrational modes on the electronic transport is discussed as well as the role of zero-point fluctuations (ZPF).

Landauer Conductance

Conductance g $\leftrightarrow$ Elastic-scattering problem $\leftrightarrow$ Transmission probability T(E)

$$g = \underbrace{2\frac{e^2}{h}}_{g_0} T(E_f)$$

$$H = H_l + H_{\mathcal{M}} + V_{l,\mathcal{M}}, \quad l = \mathrm{L}, \mathrm{R}$$

$$\boxed{T = Tr_{\mathcal{M}}[\mathbf{G}^{\dagger}_{\mathcal{M}} \mathbf{\Gamma_R} \mathbf{G}_{\mathcal{M}} \mathbf{\Gamma_L}]}$$

$\mathbf{G}_{\mathcal{M}}$ = Green function of the scattering region including coupling to the leads

$\mathbf{\Gamma}_l$ = spectral density of $l - lead$

$$[(E + i0^+)\mathbf{1}_{\mathcal{M}} - \mathbf{H}_{\mathcal{M}} - \mathbf{\Sigma_L} - \mathbf{\Sigma_R}]\mathbf{G}_{\mathcal{M}} = \mathbf{1}$$
$$\mathbf{\Sigma}_l = \mathbf{V}^{\dagger}_{l,\mathcal{M}} \mathbf{G}_l \mathbf{V}_{l,\mathcal{M}}$$
$$\mathbf{\Gamma}_l = i[\mathbf{\Sigma}_l(E + i0^+) - \mathbf{\Sigma}_l(E + i0^-)]$$

Configurational Averages [1]

(i) Density-functional-parametrized tight-binding approach to calculate the electronic and structural properties of the molecular junction

(ii) Harmonic approximation for the lattice degrees of freedom, i.e.

$$H_{\mathrm{vib}} = \sum_{\alpha=1}^{3N} \left(\frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha}{2}\omega_\alpha^2 x_\alpha^2 \right),$$

where m_α is the reduced mass of mode α, and ω_α the corresponding mode eigenfrequency. The frequencies ω_α and mode eigenvectors e_α are determined by diagonalization of the Hessian matrix.

(iii) **Thermal fluctuations** included in two complementary ways :

1. frozen-phonon approach (FPA): the scattering region is distorted according to the phonon eigenvectors
2. Molecular dynamics simulations (MD): the atoms on the scattering region evolve in time according to the classical dynamics of a system in contact with a thermal bath. The forces are calculated quantum mechanically, however.

(iv) Average transmission probabilities:

1. FP calculations:

$$g_{\mathrm{FP}} = g_0 \langle T(E) \rangle_\alpha = g_0 \int dx_1 dx_2 .... dx_{3N} T(E; \{x_\alpha\}) P(\{x_\alpha\}),$$
$$P(\{x_\alpha\}) = \prod_\alpha \left(\frac{m_\alpha \omega_\alpha^2}{2\pi E_\alpha}\right)^{1/2} \exp\left(-\frac{m_\alpha \omega_\alpha^2}{2E_\alpha} x_\alpha^2\right).$$

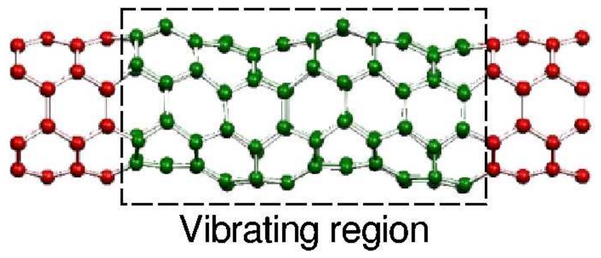
$P(\{x_\alpha\})$ is a product of gaussian distribution functions for the set of quasi-random numbers $\{x_\alpha\}$ and $E_\alpha = \hbar\omega_\alpha(N(\omega_\alpha) + 1/2)$ is the thermal energy of the α th oscillator.

2. MD simulations:

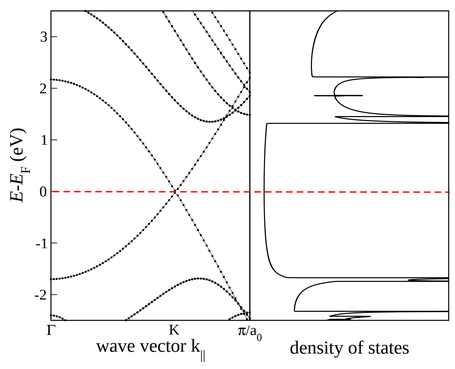
$$g_{\mathrm{MD}} = \frac{2e^2}{h} \langle T(E) \rangle_\tau = \frac{1}{\tau} \int_0^\tau dt T(E, \tau)$$

[1] *A. Pecchia et al., PRB* **68** *235321 (2003)*

Physical System: Metallic (4,4) CNT

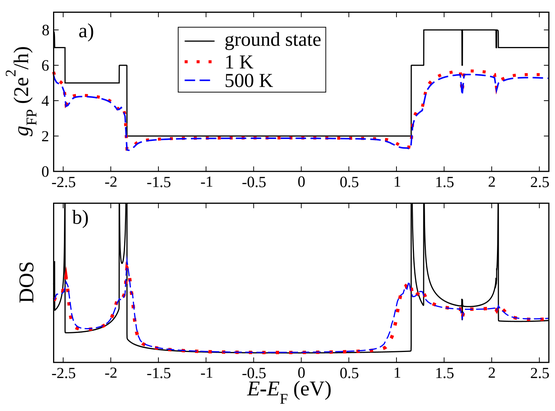


Snapshot of the vibrating scattering region (green) of the CNT. The semiinfinite contacts (red) also consist of (4,4) tubes with a **fixed** geometry.

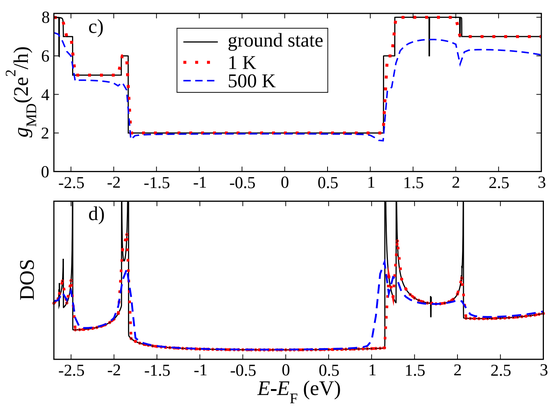


Electronic band structure and corresponding density of states (DOS) for the perfect infinite (4,4) CNT. $a_0 = 2.46\,\mathring{A}$ is the nanotube lattice constant.

FP- and MD-approaches



Average conductance in the frozen-phonon approach



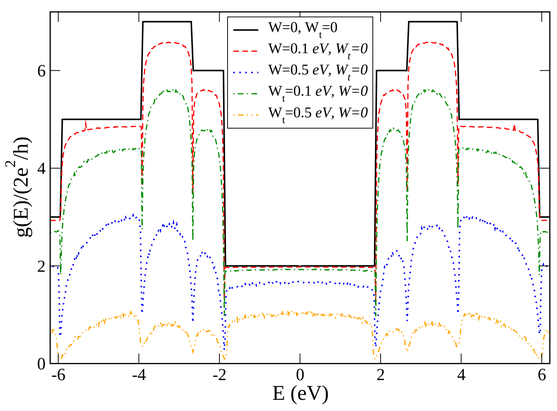
Time-averaged conductance from molecular dynamics simulations

- FPA and MD yield similar results → harmonic approximation works well for CNTs
- Zero-point fluctuations in the FPA induce sudden decrease of g_{FP} w.r.t. the static, ideal CNT conductance
- Conductance dips at the crossover points, where new bands start to contribute
- Negligible influence of structural fluctuations on the massless linear bands crossing the Fermi energy
- Strong conductance suppression on higher-lying bands related to band mixing

Static disorder

Effect of thermal fluctuations is qualitatively similar to Anderson disorder
(see also Anantram/Govindan PRB **58** 4882 (1998))

Anderson model: $H = \sum_j \epsilon_j c_j^\dagger c_j - \sum_{j,l} t_{lj}[c_j^\dagger c_l + \mathrm{H.c.}]$



Average conductance obtained from the Anderson Hamiltonian. Results for both, onsite and off-diagonal disorder are shown.

- Neglection of ZP motion increases the weight of low-frequency modes; these modes are less effective in scattering electrons → the global conductance change is less strong
- Thermal factors of high-frequency modes are basically negligible → ZP motion is dominant for them

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Single-mode analysis: Role of zero-point (ZP) motion