Spin dependent thermopower and magnetothermopower of carbon nanotube quantum dots

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Abstract

Thermopower and magnetothermopower of carbon nanotube quantum dots (CNTQs) coupled to ferromagnetic electrodes are investigated theoretically by using Green function formalism in the linear response regime. The interaction of electron-electron and electron-phonon are taken into account. Thermopower and magnetothermopower of CNTQDs are significantly affected by electron-phonon interaction. Spin thermopower and spin magnetothermopower are also studied. The results show that the (spin) magnetothermopower is increased by increase of electrodes polarization. The nonequilibrium temperature of electron and phonon subsystems and increase of electron-phonon coupling strength lead to reduction of spin magnetothermopower.

Single wall carbon nanotubes are promising candidates for fabricating nanoscale electronic device [1]. Experimental results show that carbon nanotubes with finite length act as the quantum dots [2]. Vibrational side bands within the transport spectroscopy show the presence of electron-phonon interaction (EPI) in carbon nanotube quantum dots (CNTQDs) [3]. Phonon-assisted electrical transport of CNTQD studied [4] and the influence of EPI on its thermoelectric properties has been investigated recently [5, 6]. Temperature gradient leads to thermal tunneling of electrons and induces voltage drop. On the other hand, when a magnetic field is applied on the sample or ferromagnetic (FM) electrodes coupled to the CNTQD, spin voltage drop thermally induced between electrodes is raised. We investigate the thermopower, spin thermopower, magnetothermopower (MTP) and spin magnetothermopower (SMTP) of CNTQs coupled to FM electrodes. The Influence of EPI, electron-electron interaction, is investigated by use of Green function formalism [7].

The CNTQD coupled to two electrodes can be illustrated by following Hamiltonian

$$H = \Sigma_{k\sigma}\varepsilon_{\alpha k\sigma}c^{+}_{\alpha k\sigma}c_{\alpha k\sigma} + \Sigma_{\sigma\lambda}\varepsilon_{\sigma\lambda}d^{+}_{\sigma\lambda}d_{\sigma\lambda} + \frac{U}{2}\Sigma_{\sigma'\lambda'\neq\sigma\lambda}n_{\sigma\lambda}n_{\sigma'\lambda'} + \omega a^{+}a + \Sigma_{\sigma\lambda}Mn_{\sigma\lambda}(a^{+}+a) + \Sigma_{\alpha k\sigma\lambda}[V_{\alpha k\sigma\lambda}c^{+}_{\alpha k\sigma}d_{\sigma\lambda} + H.C.], \quad (1)$$

where $c^{+}_{\alpha k\sigma}(c_{\alpha k\sigma})$ creates (destroys) an electron with spin σ, wave vector k, and energy $\varepsilon_{\alpha k\sigma}$ in the α = left (L) or right (R) electrode, $\varepsilon_{\sigma\lambda} = \varepsilon_c + \lambda\Delta_{so} + \sigma\Delta_s + V_g$ denotes energy levels of CNTQD, Δ_{so} is the spin-orbit splitting parameter and Δ_s is the spin splitting. $\sigma, \lambda = \pm 1$ denotes spin and orbit states. $d^{+}_{\sigma\lambda}(d_{\sigma\lambda})$ is the electron creation (annihilation) operator in the CNTQD. $n_{\sigma\lambda} = d^{+}_{\sigma\lambda}d_{\sigma\lambda}$ is the occupation number, whereas U is the electron-electron interaction. $a^{+}(a)$ creats (annihilates) a phonon with energyω, and M, the electron-phonon coupling strength, is dependent on the CNT diameter. $V_{\alpha k\sigma\lambda}$ is the tunneling matrix element, $\Gamma_{\alpha\sigma\lambda} = \Sigma_k\rho_{\alpha\sigma}|V_{\alpha k\sigma}|^2$ denotes spin-dependent tunneling rate and $\rho_{\alpha\sigma}$ is the electronic density of states of α electrode. We assumed $\Gamma_{\alpha\sigma\lambda} = \Gamma_0(1 \pm p_\alpha)$ is energy-independent within the wide band approximation, where Γ_0 is a constant, + (-) is for $\sigma = \uparrow (\downarrow)$, p_α denotes spin polarization of αth electrode and $p = p_L = p_R(-p_R)$ in parallel (P) (anti-parallel (AP)) configuration of electrodes. We use polaronic transformation to eliminate the electron-phonon coupling term in Hamiltonian. The imaginary part of retarded Green function of this Hamiltonian is given by [4,5,6]

$$Im\left(G^{r}_{\sigma\lambda}(\varepsilon)\right) = \Sigma_\alpha\Sigma_{n=-\infty}^{n=\infty}\frac{L_n}{\tilde{\Gamma}_{\sigma\lambda L}+\tilde{\Gamma}_{\sigma\lambda R}}[\tilde{\Gamma}_{\sigma\lambda\alpha}f_\alpha(\varepsilon+n\omega)Im\left(\tilde{G}^{r}_{\sigma\lambda}(\varepsilon+n\omega)\right) + \tilde{\Gamma}_{\sigma\lambda\alpha}(1 - f_\alpha(\varepsilon-n\omega))Im\left(\tilde{G}^{r}_{\sigma\lambda}(\varepsilon-n\omega)\right)], \quad (2)$$

and

$$L_n = e^{\frac{M}{\omega^2}(1+2N)}\left(\frac{N+1}{N}\right)^{\frac{n}{2}} I_n\left(2g\sqrt{N(N+1)}\right), \qquad (3)$$

where, $N = \left(\exp(\omega/kT_{ph}) - 1\right)^{-1}$ denotes the average phonon number, kT_{ph} is the phonon thermal energy, I_n is the first kind of Bessel function, $\tilde{G}^r_{\sigma\lambda}$ is the retarded Green function of the electronic part of Hamiltonian, $f_\alpha = (1+\exp((\varepsilon-\mu_\alpha)/kT_{e\alpha}))^{-1}$ denotes Fermi distribution function, $kT_{e\alpha}$ and μ_α are the electron thermal energy and chemical potential of α electrode. In order to compute (spin) thermopower of system, we assumed that the temperature and voltage difference between electrodes is zero. Therefore, $S = -\frac{1}{2eT_e}\left(\frac{L_{1\uparrow}}{L_{0\uparrow}} + \frac{L_{1\downarrow}}{L_{0\downarrow}}\right)$ denotes the thermopower and the spin thermopower is $S_s = -\frac{1}{2eT_e}\left(\frac{L_{1\uparrow}}{L_{0\uparrow}} - \frac{L_{1\downarrow}}{L_{0\downarrow}}\right)$, where $L_{\beta\sigma} = \int d\varepsilon\, T_{\sigma\lambda}(\varepsilon)(-\partial f/\partial\varepsilon)(\varepsilon-\mu)^\beta$, and the transmission coefficient: $T_{\sigma\lambda}(\varepsilon) = \frac{\Gamma_{\lambda\sigma L}\Gamma_{\lambda\sigma R}}{(\Gamma_{\lambda\sigma L}+\Gamma_{\lambda\sigma R})}\, Im(G^r_{\sigma\lambda}(\varepsilon))$. $MTP = (S_{AP} - S_p)/S_{AP}$ and $SMTP = (S_{S_{AP}} - S_{S_P})/S_{S_{AP}}$, where S_P (S_{AP}) denotes the thermopower of P (AP) configuration of electrodes. In numerical calculation, the electrode half band width, D, is used as energy unit, we assumed that $\omega = D/50$ and $\Gamma_0 = \omega/5$, $\Delta_{SO} = \omega$, $\Delta_s = 2\omega$, $kT_e = \omega/2$.

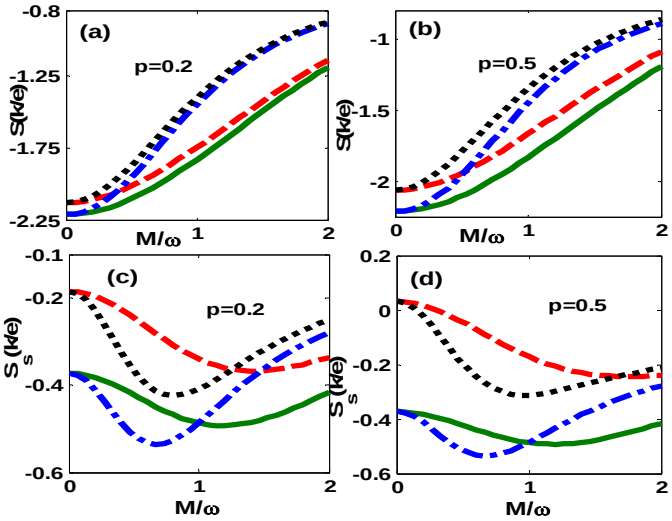

Fig1: (a) and (b) Thermopower, (c) and (d) spin thermopower of CNTQD versus electron-phonon coupling strength. Solid ($T_{ph} = T_e$) and dash-dotted ($T_{ph} = 2T_e$) lines show AP configuration, while dashed($T_{ph} = T_e$) and dotted ($T_{ph} = 2T_e$) lines are for P configuration.

The amount of CNTQD thermopower is decreased by increase of electron-phonon coupling strength, M, because the presence of EPI results in appearance of some vibrational side bands in density of states of the CNTQD. The number of these vibrational side bands increases by M and they are located far from the electrodes chemical potential ($\mu = 0$) and out of nonzero region of Fermi distribution derivative which is an important term in $L_{1\sigma}$ integral. Fig.1 shows that the values of thermopower of AP configuration of electrodes are more than P one, because in P alignment the spin-up and spin-down levels of CNTQD are attached to the left and right electrodes symmetrically. Inequality of the electron and phonon heat capacities leads to the temperature difference between electron and phonon subsystems. In the absence of EPI, the increase of phonon temperature does not change the thermopower but it reduces from equilibrium case by increase of electron-phonon coupling strength (compare dash-dotted (dotted) and solid (dashed) lines). The increase of temperature gives rise to the suppression of the thermal tunneling of electrons near the chemical potential of electrodes. The spin thermopower of AP configuration is more than P configuration

similar to the thermopower (see Fig.1 (b, c)). The results show that the increase of EPI results in increment of spin thermopower when $M < \omega$ (see solid and dashed lines), then it is slowly reduced by the increase of the EPI, because the difference between $S_{\uparrow}$and $S_{\downarrow}$is significantly dependent on the EPI. In nonequilibrium electron and phonon temperatures, the maximum amount of spin thermopower is increased and it is located in the weaker EPI, after this maximum amount the spin thermopower is reduced rapidly, because the increase of M with higher phonon temperature results in the reduction of the side bands of the density of states in the vicinity of electrodes chemical potential.

Fig. 2 shows that the MTP and SMTP are increased by increase of spin polarization of electrodes. On the other hand, we observe an increase and a decrease in MTP because the difference between P and AP configuration is affected by the EPI. When the nonequilibrium electron and phonon temperatures are considered, the MTP is reduced rapidly at high EPI, therefore, the difference between S_{AP} and S_P is reduced. The SMTP is reduced by increase of the EPI, therefore, thermal spin tunneling from electrodes to the CNTQD is suppressed by the EPI. Nonequilibrium electron and phonon temperatures result in the reduction of STMP because the difference between $S_{S_{AP}}$ and S_{S_P} is less than equilibrium condition.

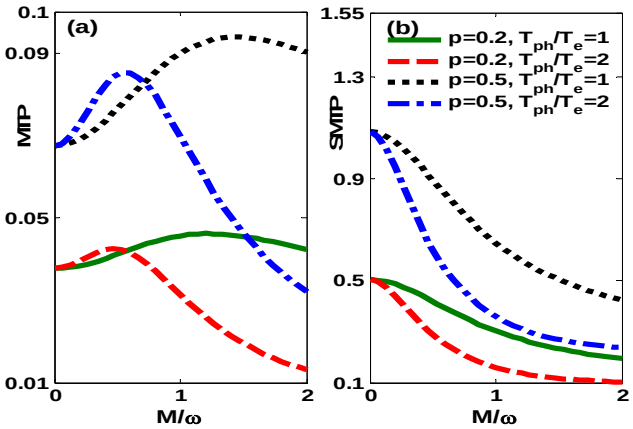

Fig. 2: (a) MTP (b) SMTP of CNTQD versus M/ω.

Conclusion

Thermopower, spin thermopower, magnetothermopower (MTP) and spin magnetothermopower (SMTP) of a carbon nanotube quantum dot coupled to the ferromagnetic electrodes are investigated theoretically by means of Green function formalism in the linear response regime. We focus on the effect of EPI and thermally nonequilibrium electron and phonon subspaces. The results show that the increase of spin polarization of electrodes increases the thermal spin tunneling of electrons through the device. On the other hand, the EPI results in the decrease of the SMTP, while the MTP is decreased by the EPI, at high electron-phonon coupling strength.

References

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