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Effect of a superconducting lead on heat generation in a quantum dot

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By using the nonequilibrium Keldysh Green's functions, we study the heat generation in a quantum dot coupled to a normal and a superconducting lead. It is found that the magnitude of the superconducting energy gap plays a crucial role in the characteristics of heat generation. For example, the local heating induced by phonon assisted Andreev reflection increases hundredfold as the gap grows from below half phonon energy $0.5\omega_0$ to above $0.5\omega_0$. Another example is the heat in the QD can be taken away efficiently only when the gap is larger than one phonon energy. It is also found that at low temperature ($T \ll \omega_0$) there exists a threshold bias voltage of half one phonon energy.

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In recent years, the local heating in nanoscale junctions has attracted a lot of attention because of the vast progress in nanofabrication. In such junctions, Joule heating arises from the interaction between electrons and phonons, which has been observed experimentally [1–4] and found to be such substantial that it poses a serious stability issue in electronic nanodevices. For a nanoscale junction, heat conduction is quite difficult. In order to prevent its stability from being jeopardized, many works have done both experimentally and theoretically [5–11] to uncover laws of local heating in nanodevices, and then find out ways to suppress the heating. On this topic, the hybrid system consisting of a quantum dot (QD) coupled to two normal leads has been investigated extensively [5–9,11,12]. Some amazing properties unique in the nanosystems, absent in macroscopic bulks, were found. For example, at zero temperature, with increasing electronic current the heating in the QD keeps zero as the bias voltage is less than one phonon energy. For a large fixed bias, the Joule heat is not proportional to the current. It was also found that a magnetic quantum dot can be cooled by a spin-polarized tunneling charge current [5].

In this paper, we shall discuss a slightly different setup, a normal-metal–quantum-dot–superconductor system (N–QD–S), which has been experimentally realized [13–15]. The transport properties of such a hybrid N–QD–S system has been widely studied [15–35]. In this geometry, the Andreev reflection occurs, in which an electron incident from the normal metal is reflected as a hole with a Cooper pair being created in the superconductor. For bias voltages less than the superconductor gap, the Andreev reflection dominates the transport process of the system. When the applied voltage is larger than the gap, both Andreev tunneling and normal tunneling contribute heavily to the conductance. Thanks to the existence of the energy gap of the superconducting lead, the physics of the transport process becomes much richer. To ensure such a hybrid system to work properly, the local heating should be taken seriously, which however has gained little previous attention, apart from the works of Wang [6] and Chen [7]. Wang found that the heat generation can be controlled by the gate voltage, bias and temperature. Chen focused mainly on how the local heating is affected by the Andreev reflection and quasi-particle current, respectively. In present work, we restrict our attention to finding how the superconductor gap magnitude affects the heating of this N–QD–S system.

The system under our consideration can be described by the following Hamiltonian (hereafter $e, \hbar = 1$):

$$H = H_L + H_R + H_D + H_T, \tag{1}$$

where,

$$H_L = \sum_{k,\sigma} \epsilon_{L,k} c^\dagger_{L,k\sigma} c_{L,k\sigma}, \tag{2}$$

$$H_R = \sum_{k,\sigma} \epsilon_{R,k} c^\dagger_{R,k\sigma} c_{R,k\sigma} + \Delta \sum_k (c^\dagger_{R,k\uparrow} c^\dagger_{R,-k\downarrow} + c_{R,-k\downarrow} c_{R,k\uparrow}), \tag{3}$$

$$H_D = \sum_\sigma \epsilon_d d^\dagger_\sigma d_\sigma + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + \omega_0 a^\dagger a + \lambda(a^\dagger + a) \sum_\sigma d^\dagger_\sigma d_\sigma, \tag{4}$$

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$$H_T = \sum_{\alpha,k\sigma} (t_\alpha c^\dagger_{\alpha,k\sigma} d_\sigma + t^*_\alpha d^\dagger_\sigma c_{\alpha,k\sigma}). \tag{5}$$

Here, H_L and H_R depict the left normal-metal and right superconducting lead, respectively, with the fermion operator $c^\dagger_{\alpha,k\sigma}$ ($c_{\alpha,k\sigma}$) ($\alpha = L, R$) creating (annihilating) an electron of vector k and spin σ ($\sigma = \uparrow, \downarrow$) in the α-lead, and 2Δ the superconducting gap. H_D is the Hamiltonian of the QD, in which the first term represents the discrete energy level in QD, the second describes the intradot electron–electron Coulomb interaction, the third is the free-phonon Hamiltonian and the last one represents the electron–phonon interaction (EPI), with $d^\dagger_\sigma$ (d_σ) and $a^\dagger$ (a) the electron and phonon creation (annihilation) operator in QD, ω_0 the phonon frequency, U and λ the strength of Coulomb repulsion and EPI. H_T denotes the tunneling Hamiltonian, where t_α represents electron hopping amplitude between QD and α-lead. For simplicity, t_α is assumed to be independent of the state k.

By coupling the QD to a large outside thermal bath, we can assume that the phonons in QD are in equilibrium Boson distribution $N_{ph} = 1/[\exp(\omega_0/\kappa_B T_{ph}) - 1]$, with T_{ph} the phonon bath temperature. Then the heat generation $Q(t)$ in the QD, i.e., energy transfer from electron reservoirs to phonon bath, per unit time at time t can be calculated from time evolution of the energy operator $E_{ph}(t) = \omega_0 n(t)$: $Q(t) = \langle d\omega_0 n(t)/dt\rangle$, where $n(t) = a^\dagger(t)a(t)$ is the phonon occupation number operator. After some algebra based on the equation of motion [8], we get

$$Q = \omega_0\lambda^2[iG^<_{DD}(\omega_0) + 2N_{ph}\mathrm{Im}\, G^r_{DD}(\omega_0)], \tag{6}$$

where $G^{</r}_{DD}(\omega_0)$ are the Fourier transformation of the lesser and retarded components of the electronic two-particle Green's function for QD: $G^<_{DD}(t,t') = -i\langle D^\dagger(t')D(t)\rangle$, $G^r_{DD}(t,t') = -i\theta(t-t')\langle[D(t), D^\dagger(t')]\rangle$, with $D(t) = \sum_\sigma d^\dagger_\sigma(t) d_\sigma(t)$.

In order to solve for the two-particle Green's functions in Eq. (6), we make a canonical transformation $\widetilde{H} = VHV^\dagger$, with the unitary operator $V = \exp[\lambda/\omega_0(a^\dagger - a)\sum_\sigma d^\dagger_\sigma d_\sigma]$. Under this transformation, the Hamiltonians for leads keep unchanged, but the Hamiltonians for QD and for electronic coupling between QD and leads become

$$\widetilde{H}_D = VH_DV^\dagger = \sum_\sigma \tilde{\epsilon}_d d^\dagger_\sigma d_\sigma + \widetilde{U} d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + \omega_0 a^\dagger a, \tag{7}$$

and

$$\widetilde{H}_T = VH_TV^\dagger = \sum_{\alpha,k\sigma} (\widetilde{V}_\alpha c^\dagger_{\alpha,k\sigma} d_\sigma + \widetilde{V}^\dagger_\alpha d^\dagger_\sigma c_{\alpha,k\sigma}). \tag{8}$$

Due to the EPI, the energy level of QD is turned into $\tilde{\epsilon}_d = \epsilon_d - \lambda^2/\omega_0$, while the charging energy $\widetilde{U} = U - 2\lambda^2/\omega_0$ and the coupling strength $\tilde{t}_\alpha = t_\alpha X$. The operator $X = \exp[-\lambda/\omega_0(a^\dagger - a)]$ arises from the canonical transformation of the electron operator $\tilde{d}_\sigma = Vd_\sigma V^\dagger = d_\sigma X$. When the EPI in QD is much stronger than electronic coupling between QD and leads, i.e., $\lambda \gg t_\alpha$, it is reasonable to replace the operator X approximately with its expectation value $\langle X\rangle = \exp[-(\lambda/\omega_0)^2(N_{ph} + 1/2)]$ [7–9,11,36]. Under this approximation, the electron–phonon interaction in QD is decoupled. For simplicity, we consider the case of $\widetilde{U} = 0$. Then the two-particle Green's functions in Eq. (6) can be transformed into product of single-particle Green's functions with the help of Wick's theorem, and the Q becomes

$$Q = \omega_0\lambda^2 \sum_{\sigma,\sigma'} \int \frac{d\omega}{2\pi} \Big\{ \widetilde{G}^<_{\sigma\sigma'}(\omega)\widetilde{G}^>_{\sigma'\sigma}(\omega - \omega_0) - 2N_{ph} \times \mathrm{Re}\Big[\widetilde{G}^r_{\sigma\sigma'}(\omega)\widetilde{G}^<_{\sigma'\sigma}(\omega-\omega_0) + \widetilde{G}^<_{\sigma\sigma'}(\omega)\widetilde{G}^a_{\sigma'\sigma}(\omega-\omega_0)\Big]\Big\}, \tag{9}$$

where $\widetilde{G}^{</>/r/a}_{\sigma\sigma'}(\omega)$ is the Fourier transform of the electronic single-particle Green's functions for QD $\widetilde{G}^{</>/r/a}_{\sigma\sigma'}(t,t')$, which are defined as $\widetilde{G}^{r/a}_{\sigma\sigma'}(t,t') = \mp i\theta(\pm t \mp t')\langle\{d_\sigma(t), d^\dagger_{\sigma'}(t')\}\rangle$, $\widetilde{G}^<_{\sigma\sigma'}(t,t') = i\langle d^\dagger_{\sigma'}(t')d_\sigma(t)\rangle$, $\widetilde{G}^>_{\sigma\sigma'}(t,t') = -i\langle d_\sigma(t)d^\dagger_{\sigma'}(t')\rangle$ and governed by the transformed Hamiltonian $\widetilde{H}$. With the help of the equation-of-motion technique, the retarded Green's function can be analytically evaluated as

$$\widetilde{G}^r_{\sigma\sigma'}(\omega) = \delta_{\sigma\sigma'}\left\{ {g^r_{11\sigma}}^{-1} - \Sigma^r_{11} - \frac{\Sigma^r_{12}\Sigma^r_{21}}{{g^r_{22\sigma}}^{-1} - \Sigma^r_{22}} \right\}^{-1}, \tag{10}$$

where ${g^r_{jj\sigma}}^{-1} = \omega + (-1)^j\tilde{\epsilon}_d + i0^+$ ($j = 1, 2$), $\Sigma^r_{11} = \Sigma^r_{22} = -i\widetilde{\Gamma}_L/2 - i\gamma(\omega)\widetilde{\Gamma}_R/2$, $\Sigma^r_{12} = \Sigma^r_{21} = i\Delta\gamma(\omega)\widetilde{\Gamma}_R/2\omega$, with $\gamma(\omega) = |\omega|/\sqrt{\omega^2 - \Delta^2}$ for $|\omega| > \Delta$ and $\gamma(\omega) = -i\omega/\sqrt{\Delta^2 - \omega^2}$ for $|\omega| < \Delta$, $\widetilde{\Gamma}_\alpha = \langle X\rangle^2\Gamma_\alpha = 2\pi\langle X\rangle^2\Sigma_k|t_\alpha|^2\delta(\omega - \epsilon_{\alpha,k})$ being the effective linewidth and assumed to be independent of energy. The advanced component is $\widetilde{G}^a_{\sigma\sigma'}(\omega) = \widetilde{G}^{r*}_{\sigma\sigma'}(\omega)$. The lesser (greater) Green's function $\widetilde{G}^{</>}_{\sigma\sigma'}(\omega)$ is proportional to the spectral function $A(\omega) = i[\widetilde{G}^r_{\sigma\sigma'}(\omega) - \widetilde{G}^a_{\sigma\sigma'}(\omega)]$ [37]. Now, the Eq. (9) can be simplified into

$$Q = 2\omega_0\lambda^2 \int \frac{d\omega}{2\pi}\big\{(N_{ph}+1)\widetilde{G}^<_{\uparrow\uparrow}(\omega)\widetilde{G}^>_{\uparrow\uparrow}(\omega-\omega_0) - N_{ph}\widetilde{G}^>_{\uparrow\uparrow}(\omega)\widetilde{G}^<_{\uparrow\uparrow}(\omega-\omega_0)\big\}. \tag{11}$$

To facilitate calculation, we introduce the 2×2 matrix Green's functions in Nambu space $\widetilde{\mathbf{G}}^{r/a}(t,t')$ and $\widetilde{\mathbf{G}}^<(t,t')$:

$$\widetilde{\mathbf{G}}^{r/a}(t,t') = \mp i\theta(\pm t \mp t') \times \begin{pmatrix} \langle\{d_\uparrow(t), d^\dagger_\uparrow(t')\}\rangle & \langle\{d_\uparrow(t), d_\downarrow(t')\}\rangle \\ \langle\{d^\dagger_\downarrow(t), d^\dagger_\uparrow(t')\}\rangle & \langle\{d^\dagger_\downarrow(t), d_\downarrow(t')\}\rangle \end{pmatrix}, \tag{12}$$

$$\widetilde{\mathbf{G}}^<(t,t') = i\begin{pmatrix} \langle d^\dagger_\uparrow(t')d_\uparrow(t)\rangle & \langle d_\downarrow(t')d_\uparrow(t)\rangle \\ \langle d^\dagger_\uparrow(t')d^\dagger_\downarrow(t)\rangle & \langle d_\downarrow(t')d^\dagger_\downarrow(t)\rangle \end{pmatrix}. \tag{13}$$

The Green's function $\widetilde{\mathbf{G}}^<_{11}(\omega)$, i.e., $\widetilde{G}^<_{\uparrow\uparrow}(\omega)$, can be solved with the help of the Keldysh equation $\widetilde{\mathbf{G}}^< = \widetilde{\mathbf{G}}^r\widetilde{\mathbf{\Sigma}}^<\widetilde{\mathbf{G}}^a$ [37], in which the lesser self-energy $\widetilde{\mathbf{\Sigma}}^<$ can be easily obtained for the case of $V_R = 0$ (V_R is voltage dropped on the right superconducting lead) as

$$\widetilde{\mathbf{\Sigma}}^<(\omega) = i\widetilde{\Gamma}_R f_R(\omega)\frac{|\omega|\theta(|\omega| - \Delta)}{\sqrt{\omega^2 - \Delta^2}}\begin{pmatrix} 1 & -\Delta/\omega \\ -\Delta/\omega & 1 \end{pmatrix} + i\widetilde{\Gamma}_L\begin{pmatrix} f_L(\omega + eV_L) & 0 \\ 0 & f_L(\omega - eV_L) \end{pmatrix}, \tag{14}$$

where, we have assumed t_α to be real for simplicity. $f_\alpha(x) = [\exp(x/\kappa_B T_\alpha) + 1]^{-1}$ is the Fermi distribution function with T_α temperature of the α-lead, and V_L is the voltage of the left normal lead. Substituting the lesser self-energy $\widetilde{\mathbf{\Sigma}}^<(\omega)$, Eq. (14), into the Keldysh equation, we obtain

$$\widetilde{\mathbf{G}}^<_{11}(\omega) = i\widetilde{\Gamma}_L\Big[|\widetilde{\mathbf{G}}^r_{11}(\omega)|^2 f_L(\omega + eV_L) + |\widetilde{\mathbf{G}}^r_{12}(\omega)|^2 f_L(\omega - eV_L)\Big] + i\widetilde{\Gamma}_R f_R(\omega)\frac{|\omega|\theta(|\omega| - \Delta)}{\sqrt{\omega^2 - \Delta^2}}\Big\{|\widetilde{\mathbf{G}}^r_{11}(\omega)|^2 + |\widetilde{\mathbf{G}}^r_{12}(\omega)|^2 - \frac{2\Delta}{\omega}\mathrm{Re}\Big[\widetilde{\mathbf{G}}^r_{11}(\omega)\widetilde{\mathbf{G}}^{r*}_{12}(\omega)\Big]\Big\}, \tag{15}$$

where the retarded Green's function $\widetilde{\mathbf{G}}^r_{11}(\omega)$, i.e., $\widetilde{G}^r_{\uparrow\uparrow}(\omega)$, is given by Eq. (10), and

$$\widetilde{\mathbf{G}}^r_{12}(\omega) = \widetilde{\mathbf{G}}^r_{11}(\omega)\gamma(\omega)\widetilde{\Gamma}_R\Delta\frac{i}{2\omega} \times \left[\omega + \tilde{\epsilon}_d + \frac{i}{2}\widetilde{\Gamma}_L + \frac{i}{2}\gamma(\omega)\widetilde{\Gamma}_R\right]^{-1}. \tag{16}$$

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