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<th><strong>Title</strong></th>
<th>Optimal quantum pump in the presence of a superconducting lead</th>
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Since the seminar work of Thouless\textsuperscript{1} and Brouwer,\textsuperscript{2} the physics of parametric pumping has attracted increasing attention.\textsuperscript{3–18} Recently, Avron \textit{et al}.,\textsuperscript{19} have considered the heat current generated by the pump in the adiabatic regime and found a general lower bound for the heat current. This defines an optimal pump if the heat current equals to the power of Joule heat dissipated during the pumping process.\textsuperscript{19} As a consequence, the optimal pump is noiseless and the charge transported is quantized. The physics of heat current has also been investigated by Moskalets and Buttiker\textsuperscript{20} who have derived a general formula for the heat current in the weak pumping regime and the noise generated during the pumping process.\textsuperscript{20} For chaotic quantum dots, Polianski \textit{et al}.,\textsuperscript{22} have developed a time-dependent scattering matrix theory to account for the noise for parametric pumping and mesoscopic fluctuation for arbitrary temperature and beyond bilinear response. In this paper, we investigate the pumped heat current for a normal superconducting (NS) hybrid system that consists of a normal quantum dot, a normal lead, and a superconducting lead. In the adiabatic regime, the energy of charged carriers (electron or hole) is within the superconducting energy gap and hence physics of the Andreev reflection\textsuperscript{23} dominates. We have derived a general expression for the pumped electric current and heat current in the presence of a superconducting lead which is valid at finite pumping amplitude and finite temperature. Our theory is based on the time-dependent scattering matrix theory.\textsuperscript{10} Going beyond the adiabatic regime, we can in principle obtain the pumped electric current and heat current to any order in frequency. In the adiabatic regime, we have also derived a relationship among the instantaneous heat current, electric current, and the noise. This sets a lower bound for the heat current generated by the pump. Similar to the normal system,\textsuperscript{19} a quantum pump will be optimal if the heat current reaches its lower bound. As a result, the charge transported will be quantized and the system is noiseless just like the normal system. We have also compared with the heat current of NS structure with that of normal structure. For a single pumping potential, the total heat currents generated are the same for NS and normal systems. For two pumping potentials the heat current for NS system can be either larger or smaller than that of normal system depending on the phase difference between two pumping potentials.

For the purpose of presentation, we consider the pumped electric current first. We start with the general definition for the electric current of type $\alpha$ (electron or hole) in the left lead,\textsuperscript{19}

$$I_{e,\alpha} = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_0^{\Delta t} dt \langle \hat{I}_{e,\alpha} \rangle,$$

where $\langle \cdots \rangle$ denotes the quantum average and $\hat{I}_{e,\alpha}$ is the electric current operator of type $\alpha$ in the left lead,

$$\hat{I}_{e,\alpha} = q_\alpha \left( \hat{b}_{\alpha,\text{L}}(t) \hat{b}_{\alpha,\text{L}}(t) - \hat{a}_{\alpha,\text{L}}(t) \hat{a}_{\alpha,\text{L}}(t) \right).$$

Here the operators $\hat{b}_{\alpha,\text{L}}$ and $\hat{a}_{\alpha,\text{L}}$ are annihilation operators for the outgoing and incoming carriers of type $\alpha$ in the left lead and $q_\alpha = 1, -1$ for $\alpha = e, h$. They are related by the scattering matrix\textsuperscript{20,26}

$$\hat{b}_{\alpha,\text{L}}(t) = \sum_{\beta} \int dt' S_{\alpha\beta}(t, t') \hat{a}_{\beta,\text{L}}(t'),$$

where the time dependence of the scattering matrix $S$ is due to the slowly time-varying pumping potential $X(t)$. The distribution function can be obtained by taking the quantum average,\textsuperscript{20}

$$\langle \hat{a}_{\alpha,\text{L}}(E) \hat{a}_{\beta,\text{L}}(E') \rangle = \delta_{\alpha\beta} \delta(E - E') f_L(E),$$

where $\hat{a}_{\alpha,\text{L}}(E)$ is the Fourier transform of $\hat{a}_{\alpha,\text{L}}(t)$, and $f_L(E)$ is the Fermi distribution function of the left lead. From Eqs. (2)–(4), the pumped electric current is given by

$$I_{e,\alpha} = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_0^{\Delta t} dt \int dt_1 dt_2 \sum_{\beta} S_{\alpha\beta}(t, t_1)
\times f(t_1 - t_2) S_{\alpha\beta}^{*}(t_2, t_1) - q_\alpha \int \frac{dE}{2\pi} f(E),$$

where $f(t) = \int (dE/2\pi) \exp(-iEt)f(E)$. After changing of the variables $t_0 = (t_1 + t_2)/2$ and $\tau = t_1 - t_2$, and using the following Wigner transform for the scattering matrix,\textsuperscript{28}
\[ S(t,t') = \int \frac{dE}{2\pi} e^{-iE(t-t')} S\left( E, \frac{t+t'}{2} \right), \]  

(6)

Eq. (5) becomes

\[ I_{e,L.a} = \lim_{\Delta t \to 0} -q_a 4\pi i \int \frac{d\tau}{\Delta t} \int dt_0 d\tau \delta E_1 dE_2 f(\tau) \]

\[ \times e^{-iE(t-t_0-\tau/2)} e^{iE_2(t-t_0+\tau/2)} \sum_\beta S_{\alpha\beta}(E_1, \frac{t+t_0}{2}) \]

\[ + \frac{\tau}{4} \times S^*_{\alpha\beta}(E_2, \frac{t+t_0}{2} - \frac{\tau}{4}) - q_a \int \frac{dE}{2\pi} f(E). \]  

(7)

Changing the variables again to \( \tau_1 = t-t_0 \) and \( t' = (t+t_0)/2 \) and integrating over \( \tau_1 \), we obtain

\[ I_{e,L.a} = \lim_{\Delta t \to 0} -q_a \frac{q_a}{2\pi \Delta t} \int \frac{d\tau'}{\Delta t} \int dt \delta E e^{iE \tau} f(\tau) \]

\[ \times \sum_\beta S_{\alpha\beta}(E,t') + \tau/4) S^*_{\alpha\beta}(E,t' - \tau/4) - q_a \]

\[ \times \int \frac{dE}{2\pi} f(E). \]  

(8)

Using the fact that

\[ \lim_{\Delta t \to 0} \int_{\tau_0}^{\tau_1} \int dt' \sum_\beta S_{\alpha\beta}(E,t' + \tau/4) S^*_{\alpha\beta}(E,t' - \tau/4) \]

\[ = \lim_{\Delta t \to 0} \int \frac{\Delta t}{\tau_0} \int dt \sum_\beta S_{\alpha\beta}(E,t) e^{-(\tau_0)/2} S^*_{\alpha\beta}(E,t_1). \]  

(9)

Eq. (8) becomes

\[ I_{e,L.a} = \frac{q_a}{\pi T_p} \int_0^{T_p} dt \int dE \{ \hat{S}(E,t) \}

\[ \times [f(E+i\partial/2) - f(E)] \hat{S}^*(E,t) \}_{aa}. \]  

(10)

where \( T_p \) is the period of the pumping cycle and \( \hat{S} \) is a \( 2 \times 2 \) scattering matrix for NS structure with matrix element \( S_{\alpha\beta}(\alpha, \beta = e, h) \). Equation (10) is symbolic and is the central result of this paper. One can in principle obtain the pumped electric current to any order in frequency. For instance, to get the electric current up to \( \omega \), it is enough to expand \( f(E + i\partial/2) \) up to the first order in \( \partial \), from which we obtain

\[ I_{e,L.a} = \frac{iq_a}{\pi T_p} \int_0^{T_p} dt \int dE \hat{S}(E,t) \]

\[ \times \{ f(E+\partial/2) - f(E) \} \hat{S}^*(E,t) \}_{aa}. \]  

(11)

Note that from the unitary condition of the scattering matrix \( \hat{S} \), we have

\[ \sum_\beta S^*_{\alpha\beta} S_{\alpha\beta} = 1. \]  

(12)

Taking the derivative with respect to time, we obtain

\[ \sum_\beta \partial_t S^*_{\alpha\beta} S_{\alpha\beta} + c.c. = 0. \]  

(13)

Hence \( \text{Im}[i(\partial_t \hat{S})_{aa}] = -i(\partial_t \hat{S})_{aa} \). In the adiabatic regime, we have \( \hat{S}_{\alpha\beta} = \sum_i (\partial X_i \hat{S}_{\alpha\beta} \delta X_i + \hat{S}_{\alpha\beta} \partial X_i \delta X_i + \cdots) \). Therefore, we can neglect the contribution from \( \partial X_i \delta X_{\alpha\beta} \). At zero temperature, Eq. (11) becomes

\[ I_{e,L.a} = \frac{iq_a}{2\pi T_p} \int_0^{T_p} dt [\partial_{X_i} \hat{S}^*(E,t)]_{aa} \hat{S}_{\alpha\beta} \delta X_i, \]  

(14)

which agrees with the theory of nonequilibrium Green’s function.27

Now we proceed to derive the heat current generated by the pump for NS structure. We note that the heat current is defined as the particle current multiplied by the energy measured from the Fermi level. We thus have from Eq. (10),

\[ I_{q,L.a} = \frac{1}{\pi T_p} \int_0^{T_p} dt \int dE (E - E_F) \{ \hat{S}(E,t) \}

\[ \times [f(E+i\partial/2) - f(E)] \hat{S}^*(E,t) \}_{aa}. \]  

(15)

Expanding the heat current up to \( \partial^2 \) and after some algebra, we finally obtained the heat current up to \( \partial^2 \),

\[ I_{q,L.a} = -\frac{1}{8 \pi T_p} \int_0^{T_p} dt \int dE \hat{S}_E f(\partial \hat{S} \partial \hat{S}) \}_{aa}. \]  

(16)

Now we derive the relationship between instantaneous electric current [denoted as \( I_{e}(t) = -i(q_a \partial_t \hat{S})_{aa} \)] and heat current [\( I_{q}(t) = \partial S^t \partial H S \)]. Now the instantaneous heat current becomes

\[ I_{q}(t) = (\partial_t \hat{S}^t \partial H \hat{S})_{aa} = (\partial_t \hat{S}^t \hat{S} \partial H \hat{S})_{aa} \]

\[ = \sum_\beta (\partial_t \hat{S}^t \hat{S})_{\alpha\beta} (\partial H \hat{S})_{\alpha\beta} \]  

(17)

We see that the diagonal term in Eq. (17) is just \( I^2_{e}(t) \) and the off-diagonal term is the noise \( S_0(t) \) generated during the pumping process. Therefore, we have the following relationship:

\[ I_{q}(t) = I^2_{e}(t) + S_0(t) \]  

(18)

or general lower bound for the heat current

\[ I_{q}(t) \geq I^2_{e}(t). \]  

(19)

The condition of optimal pump for NS structure is defined as \( S_0(t) = 0 \). Following Avron et al., it is straightforward to show that the charge transported through the system per cycle is quantized if the quantum pump is optimal.

Now we consider the adiabatic and weak pumping limit for a symmetric double-barrier structure in the presence of superconducting lead. The double-barrier structure is modeled by potential \( V(x) = X_1(t) \delta(x+a) + X_2(t) \delta(x-a) \), where \( X_1(t) = X_0 + X_1 \sin(\omega t) \) and \( X_2(t) = X_0 + X_2 \sin(\omega t) \).
+ \phi). In this limit, we keep only the quadratic order in pumping amplitude in Eqs. (14) and (16). It is easy to show that the pumped electric current and heat current are given, respectively, by

$$I_{e,La} = \frac{\omega q_s \sin \phi X_2 X_3}{2\pi} \text{Im}[(\partial_{x_2} S_1^a \partial_{x_1} S_2^a)_{aa}]$$  \hspace{1cm} (20)

and

$$I_{q,La} = \frac{\omega^2}{16\pi} \left[ X_1^2 \partial_{x_1} S_1^a \partial_{x_1} S_1^a \partial_{x_2} S_1^a \partial_{x_2} S_1^a + 2 \cos \phi X_1 X_2 \text{Re}(\partial_{x_1} S_{\alpha 2} \partial_{x_2} S_{\alpha 1}^\dagger) \right]_{aa}.$$  \hspace{1cm} (21)

In Eqs. (20) and (21), we have set $X_1 = 0$ in $S$ after the partial derivatives. Now we will calculate the heat current $I_{q,La=\epsilon}$ for the double-barrier NS system. For the NS system, the scattering matrices $S_{ee}$ and $S_{he}$ are given by\textsuperscript{23,29}

$$\hat{S} = S_{11} + S_{12}(1 - R_{1f} S_{22})^{-1} R_{1f} S_{21},$$  \hspace{1cm} (22)

where

$$\hat{S}_{ij}(E) = \begin{pmatrix} S_{ij}(E) & 0 \\ 0 & S_{ij}(-E) \end{pmatrix},$$  \hspace{1cm} (23)

with $S_{ij}$ being usual scattering matrix for the normal structure. $R_{1f}$ is the $2 \times 2$ scattering matrix at NS interface with off-diagonal matrix element $\alpha \epsilon$. Here $\alpha = (E - i \nu \sqrt{\Delta^2 - E^2})/\Delta$ with $\nu = 1$ when $E > -\Delta$ and $\nu = -1$ when $E < -\Delta$. In Eq. (22), the energy $E$ is measured relative to the chemical potential $\mu$ of the superconducting lead. Equation (22) has clear physical meaning.\textsuperscript{29} The first term is the direct reflection from the normal scattering structure and the second term can be expanded as $\hat{S}_{12} R_{1f} \hat{S}_{21} + S_{12} R_{1f} S_{22} R_{1f} \hat{S}_{21} + \cdots$, which is clearly the multiple Andreev reflection in the hybrid structure. From Eq. (22) we obtain the well-known expressions for the scattering matrices $S_{ee}$ and $S_{he}$,\textsuperscript{23}

$$S_{ee}(E) = S_{11}(E) + \alpha^2 S_{12}(E) S_{22}^{\dagger}(-E) M_e S_{21}(E)$$  \hspace{1cm} (24)

and

$$S_{he}(E) = \alpha S_{12}^{\dagger}(-E) M_e S_{21}(E),$$  \hspace{1cm} (25)

with $M_e = [1 - \alpha^2 S_{22}(E) S_{22}^{\dagger}(-E)]^{-1}$. In the case of parametric pumping, we assume that the Fermi energy is in line with the chemical potential of superconducting lead, so $E = 0$ and $\alpha = -i$. For the symmetric NS system at resonance, we have\textsuperscript{9} $S_{11} = 0$ and $S_{12} = e^{-2i \epsilon a}$ in the absence of pumping potential. Therefore, from Eqs. (24) and (25), we have

$$\partial_{x_1}^2 S_{ee} = S_{11} - S_{12}^2 \partial_{x_2} S_{21}^{\dagger}$$  \hspace{1cm} (26)

and

$$\partial_{x} S_{he} = -i(\partial_{x} S_{22} \partial_{x} S_{11} + \text{c.c.}),$$  \hspace{1cm} (27)

where we have used the fact that $\partial_{x_1} S_{22} = \partial_{x} S_{11}$. Using Fisher-Lee relation\textsuperscript{30} $S_{ab} = -\delta_{ab} \pm i \upsilon G_{ab}$ and the Dyson equation $\partial_{x} G_{\alpha \beta} = G_{\alpha \beta} G_{\beta \gamma} G_{\gamma \alpha}$, we have

$$\partial_{x_1} S_{11} = i \upsilon G_{11}, \quad \partial_{x_2} S_{22} = -i \upsilon G_{22}, \quad \partial_{x_2} S_{12} = -i \upsilon G_{12}, \quad \partial_{x_2} S_{11} = -i \upsilon G_{11} G_{11},$$

$$\partial_{x_1} S_{12} = -i \upsilon G_{12} G_{12}.$$  \hspace{1cm} (28)

Hence we have

$$I_{q,La} = \frac{\omega^2}{16k^2}[X_1^2 + X_2^2 + 2 \cos \phi X_1 X_2 \cos 4 \upsilon a].$$  \hspace{1cm} (29)

We note that in the NS system, the heat current flows out only through the normal lead; while for normal system, the heat current pumps out through both leads. Comparing Eqs. (28) and (29), we have

$$I_{q,L}^N + I_{q,R}^N - I_{q,L}^N = \frac{\omega^2}{16k^2} \cos \phi X_1 X_2 (1 - \cos 4 \upsilon a).$$  \hspace{1cm} (30)

Hence the total heat current generated in the normal system can be either larger or smaller than that in the NS system depending on the phase difference of two pumping potentials. For a single pump, by setting $X_2 = 0$ in Eqs. (28) and (29), we see that the total heat currents are the same for both NS and normal systems. This is different from the pumped electric current where in the weak pumping regime at resonance, the electric current for NS system is four times larger than that of normal system.\textsuperscript{9}

In summary, we have derived a general expression for the pumped electric current and heat current in the presence of superconducting lead using the time-dependent scattering matrix theory. Our theory is valid at finite pumping amplitude and can be applied to the multichannel systems. Using our theory, we can expand Eq. (15) to higher order in frequency and hence approach to the nonadiabatic regime. Our theory can also be easily extended to the case of multiterminal structures. Although our expression is derived for NS system, it is also valid the normal system as well by simply replacing the NS scattering matrix $S_{ab}$ with $\alpha \beta = e, h$ by normal system scattering matrix $S_{ij}$ with $i, j = 1, 2$ in Eqs. (10) and (15). For the NS system, we have found the lower bound for the heat current similar to that of Avron et al.\textsuperscript{19} for the normal system. As a result, the optimal pump can exist for NS system as well. In the weak pumping limit, we have examined the heat current for NS system for a double-barrier structure at resonance. For two-parameter pump, we found that the total heat current for NS structure can be larger or smaller than that of normal structure depending on the phase different between two pumping parameters.

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24 Our theory is valid only for frequency $\omega < \Delta$. For $\omega \approx \Delta$, we have to use the nonequilibrium Green’s-function method. 25
27 There is a typo mistake in Eq. (2) of Ref. 9, where the minus sign should be the plus sign.
28 When $\hbar \omega \approx k_B T$, the noise is $S(t) = S^0_\omega(t)/(4 \pi k_B T) = |\delta s_{\omega}^0 S^*_\omega|/(4 \pi k_B T)$. It is proportional to $\omega^2$.