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HEAT CURRENTS IN NON-SUPERCONDUCTING FLUX QUBITS*

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A flux qubit based on a non-superconducting mesoscopic ring coupled to two split heat baths at different temperatures is studied. Heat currents flowing in such a nonequilibrium quantum thermodynamic system are analyzed. A method of control of heat transfer via the qubit is proposed.

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1. Introduction

Thermodynamics of macroscopic systems is a closed theory dating back to 19th century. With the development of mesoscopic and nano-physics, thermodynamics of small system based on quantum mechanics should be formulated. Indeed, in last several years, this hot topic has attracted considerable attention not only as a fundamental theory but also due to its possible application in building small heat engines, nanomachines [1] and molecular motors [2]. Because small systems (almost) always exhibit quantum character, one is faced with a non-trivial problem of thermodynamics of processes in open quantum systems [3, 4]. As statistical mechanics is "the bridge between the world of atom and the world of object" [3] designing 'building blocks' of any device essentially based on quantum properties of the Nature, one is faced with a highly non-trivial problem of modeling of quantum irreversibility.

In this paper we limit our attention to specific properties of very specific systems: heat flows through flux qubits based on non-superconducting materials [5]. The qubit is coupled to two quasi-free thermal reservoirs at different temperatures. It is obvious that any heat engine or any other machine operating with thermal energy flows is a stage of heat conductance.

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The heat currents granting desired properties of the device should be controllable. Below we show that such a control can be performed when working with recently proposed flux qubits based on non-superconducting mesoscopic rings [5]. It is demonstrated that heat currents are controllable by an externally applied magnetic field which induces the magnetic flux of the ring. The result of such a control is different for qubits build on rings accommodating even or odd number of electrons. This property of persistent currents of mesoscopic rings is absent in superconducting flux qubits [6] and therefore the former has a potential advantage for applications.

In Sec. 2, we define the model of the non-superconducting flux qubit. In Sec. 3, we present a master equation for the qubit coupled to two independent heat baths. Heat transport in the system is analyzed in Sec. 4. We end with the summary in Sec. 5.

2. Non-superconducting flux qubit

Recently a number of systems have been shown to be reducible to two-level systems [6, 7]. The aim of such a procedure is obvious: searching new candidates for qubits. The solid state devices seem to be a promising attempt. As an example one can mention superconducting charge or flux qubits [6]. In this paper we consider flux qubits based on non-superconducting materials. We follow a model developed in [5].

Let us consider a mesoscopic metallic or semiconducting quasi $1D$ ring of radius R ($2\pi R < L_\phi$, L_ϕ is the coherence length) in presence of a static magnetic flux $\phi = \pi R^2 B_e$ with B_e being an applied magnetic field perpendicular to the plane of the ring. The number of electrons maintaining the phase coherence can either be even $N = N_{\text{even}}$ or odd $N = N_{\text{odd}}$. These two cases result in different properties of the qubit [8].

We assume that the ring is made of a clean material and the transport regime is ballistic. The energy spectrum of such a ring consists of a set of well known parabolas $E_n \sim (n - \phi/\phi_0)^2$ (n integer) with the flux quantum $\phi_0 = h/e$. The spectrum becomes degenerate if the flux ϕ/ϕ_0 assumes integral (for $N = N_{\text{even}}$) or half-integral (for $N = N_{\text{odd}}$) values. This degeneracy can be removed if there is a distortion of the ring causing the potential barrier of finite length. Such a distortion can be achieved either by geometric deformation of the ring (*e.g.* by the atomic force microscope) or by an electric gating [5]. The potential barrier causes splitting of the degeneracy of the state $\{|-n_{\text{F}}\rangle, |n_{\text{F}}\rangle\}$ (for $N = N_{\text{even}}$) or the state $\{|-n_{\text{F}}\rangle, |n_{F+1}\rangle\}$ (for $N = N_{\text{odd}}$), where $|n_{\text{F}}\rangle$ denotes the energy eigenstate at the Fermi surface. Let us notice that the initially degenerate states carry persistent currents of the same amplitude but opposite sign. If the energy splitting is smaller than the energy gap Δ at the Fermi surface these states span the two dimensional Hilbert space of the qubit.

In a pseudospin notation the dimensionless Hamiltonian of such a system can be written as [5]

$$H_{\mathrm{q}} = -\tfrac{1}{2}B_z\sigma_z - \tfrac{1}{2}B_x\sigma_x \,, \tag{1}$$

where σ_z and σ_x denote Pauli spin matrices. The term B_z can be tuned by the applied magnetic flux

$$B_z = \begin{cases} \Delta\left[1 - 2\frac{\phi}{\phi_0}\right] & \text{for } N = N_{\mathrm{odd}}\,, \\ -2\Delta\frac{\phi}{\phi_0} & \text{for } N = N_{\mathrm{even}}\,, \end{cases} \tag{2}$$

leading to the possibility of an effective control. Let us notice that given external control results in different properties of qubits based on rings accommodating either even or odd number of electrons.

The x component of the effective magnetic field B_x describes the tunneling amplitude between two potential wells and can be tuned by changing the height of the potential barrier (*e.g.* electrical gating).

3. Master equation for flux qubit

In this section we present a master equation for the statistical operator $\rho(t)$ of the flux qubit interacting with two thermal baths. The thermal bath, say 1, has temperature T_1 and the bath 2 has temperature T_2. There are several various ways of derivation of master equations for quantum open systems. In practice, formally exact master equations have to be approximated (there are a few exceptions when models are exactly solvable [9]). Otherwise, they are useless. Approximated master equations can suffer from a serious shortcoming: the positivity of the statistical operator can be destroyed. Moreover, the range of its applicability is not well-defined. Here we apply rigorous Davies theory which works in the weak coupling regime [10, 11].

We start with the Hamiltonian of the total system consisting of the flux qubit Q coupled to two bosonic heat baths of temperatures T_1 and T_2, namely,

$$H = H_{\mathrm{q}} + \sum_{i=1}^{2}\left(H_{\mathrm{int}}^{(i)} + H_R^{(i)}\right)\,, \tag{3}$$

where H_{q} is the Hamiltonian (1) of the qubit. The heat baths consist of an infinite number of mutually independent harmonic oscillators,

$$H_R^{(i)} = \sum_n \omega_n^{(i)} a_n^{(i)\dagger} a_n^{(i)}\,, \qquad i = 1, 2\,. \tag{4}$$

The interaction $H_{\rm int}^{(i)}$ of the qubit with the heat baths is assumed to be linear and its form reads

$$H_{\rm int}^{(i)} = \frac{1}{2}\left(w^{(i)}\sigma_z + u^{(i)}\sigma_x\right)\sum_n c_n^{(i)}\left(a_n^{(i)} + a_n^{(i)\dagger}\right)\,, \tag{5}$$

with coupling characterized by the parameters $w^{(i)}, u^{(i)}$ and $c_n^{(i)}$. The master equation for the statistical operator $\rho(t)$ of the qubit derived via the rigorous Davies approach is given by the relation [11]

$$\dot\rho(t) = \left[D_H + D_R^{(1)} + D_R^{(2)}\right]\rho(t)\,, \tag{6}$$

where the Hamiltonian 'conservative' part takes the form

$$D_H\rho(t) = -i\left[H_{\rm q} + \sum_{i=1}^{2}\left(\sum_{k,l=1}^{2} s^{(i)}(\Omega_{kl})A_{kl}^{(i)\dagger}A_{kl}^{(i)}\right), \rho(t)\right]\,, \tag{7}$$

and the non-Hamiltonian part

$$D_R^{(i)}\rho(t) = \frac{1}{2}\left(\sum_{k,l=1}^{2} c^{(i)}(\Omega_{kl})\left(\left[A_{kl}^{(i)}\rho(t), A_{kl}^{(i)\dagger}\right] + \left[A_{kl}^{(i)}, \rho(t)A_{kl}^{(i)\dagger}\right]\right)\right)\,,\ i=1,2\,, \tag{8}$$

contains all dissipative effects. The operators of the Fourier decomposition of the interaction Hamiltonian are given by

$$A_{kl}^{(i)} = \tfrac{1}{2}P_k(w^{(i)}\sigma_z^{(i)} + u^{(i)}\sigma_x^{(i)})P_l\,, \tag{9}$$

with the following spectral representation of the flux qubit Hamiltonian:

$$H_{\rm q} = \sum_{j=1}^{2}\lambda_j P_j\,, \tag{10}$$

$$\Omega_{kl} = \lambda_l - \lambda_k\,, \tag{11}$$

where P_j are projector operators and λ_j are eigenvalues of the Hamiltonian $H_{\rm q}$.

The i-th reservoir is characterized by the frequency spectrum $J^{(i)}(\nu) = \sum_n [c_n^{(i)}]^2\delta(\nu - \omega_n^{(i)})$, which in the thermodynamic limit for the reservoir is assumed to be a smooth function. The coefficients in the master equation can then be expressed as the Fourier transform

$$c^{(i)}(\omega) = \int_{-\infty}^{\infty}\mathcal{C}^{(i)}(t)\exp(-i\omega t)dt \tag{12}$$

of the function

$$\mathcal{C}^{(i)}(t) = \int_0^\infty J^{(i)}(\nu)[\coth(\beta_i \nu/2)\cos(\nu t) + i\sin(\nu t)]d\nu\,, \tag{13}$$

where $\beta_i = 1/kT_i$, k is the Boltzmann constant and T_i is temperature of the i-th bath. One can use the Hilbert transform to obtain the coefficients $s^{(i)}(\omega)$, namely,

$$s^{(i)}(\omega) = \frac{\mathcal{P}}{2\pi}\int_{-\infty}^{\infty} \frac{c^{(i)}(\nu)}{\nu - \omega} d\nu\,. \tag{14}$$

The form of the spectral function $J^{(i)}(\nu)$ reflects not only the energies present in the environment but also the 'weights' of coupling between the qubit and the modes of the heat bath. The experimental setup applied both in experiments and theoretical considerations related either to superconducting or to non-superconducting flux qubits assumes the environment built and controlled by the SQUID device [6, 12]. The presence of the macroscopic SQUID can effectively be modeled by coupling of the qubit to the thermal bath via the operator σ_z [5, 12].

The energy barrier leading to the separation of qubit energy levels (B_x) can also be affected by fluctuations of an environment. The barrier is controlled either by means of an atomic force microscope or electrical gating [5] and fluctuates. Such an effect shall be incorporated as a second heat bath coupled by σ_x to the qubit. As both 'baths' can be spatially separated they can operate at different temperatures which results in a heat current between them. The above described coupling shall be referred as $\sigma_z\sigma_x$-coupling, *i.e.* $u^{(1)} = 0$ and $w^{(2)} = 0$ in Eq. (5). This abbreviated notation shall be intensively used trough the paper.

In the discussion we assume, following [12], that the spectral properties of both heat baths can be modeled by the ohmic dissipation, namely,

$$J^{(i)}(\nu) = \frac{\alpha^{(i)}}{2}\nu \exp(-\nu/\omega_c)\,. \tag{15}$$

The cut-off frequency ω_c determines the largest energy scale of the reservoirs (from the technical point of view, it removes possible divergences at high frequencies). The parameter $\alpha^{(i)}$ is the coupling strength of the qubit and the i-th heat bath (below we assume that $\alpha^{(1)} = \alpha^{(2)} = \alpha$). For completeness we shall also study other architectures when both baths are coupled by the same operators, *i.e.* '$\sigma_x\sigma_x$-coupling', *i.e.* $w^{(1)} = 0$ and $w^{(2)} = 0$ in Eq. (5) or '$\sigma_z\sigma_z$-coupling', *i.e.* $u^{(1)} = 0$ and $u^{(2)} = 0$ in Eq. (5).

4. Heat transport

The change of energy $E(t) = \mathrm{Tr}[H_{\mathrm{q}}\rho(t)]$ of the qubit is determined by the master equation (6),

$$\frac{dE}{dt} = J(t) = J_1(t) + J_2(t)\,. \tag{16}$$

The heat current $J_1(t)$ between the qubit and the bath 1 is defined by the energy dissipated via the first bath, namely, it is the change of energy of Q due to the coupling to the first reservoir,

$$J_1(t) = \mathrm{Tr}[H_{\mathrm{q}} D_R^{(1)} \rho(t)]\,, \tag{17}$$

where the dissipator $D_R^{(1)}$ is given by Eq. (8). *Mutatis mutandis*, the heat current $J_2(t)$ between the qubit and the bath 2 is given by the relation

$$J_2(t) = \mathrm{Tr}[H_{\mathrm{q}} D_R^{(2)} \rho(t)]\,, \tag{18}$$

with the dissipator $D_R^{(2)}$ in Eq. (8). Let us assume that $T_1 < T_2$. In the thermalization process, no work is performed, but heat is exchanged between the baths 1 and 2 via the qubit. This process is an information-erasure process. In the stationary state, when $t \to \infty$, the statistical operator $\rho(t) \to \rho$ and the total heat current $J(t) \to J = J_1 + J_2 = 0$. Moreover, because $T_2 > T_1$, the stationary heat current $J_2 > 0$ (heat is flowing from the reservoir 2 to the qubit) and $J_1 < 0$ (heat is flowing from the qubit to the reservoir 1). Therefore the qubit can be viewed as a 'mesoscopic bridge' generating a stationary leakage current $J_2 = -J_1$.

We show that such a system is effectively controllable by the applied magnetic flux which, except temperature, is the main control parameter. The magnetic flux enters the system Hamiltonian via B_z in H_{q}, *cf.* Eq. (1). Because of the dependence of B_z on the number of electrons, *cf.* Eq. (2), the results for qubits built on rings with even and odd numbers of electrons can be substantially different. To be more concrete, let us assume that initially the qubit is prepared in the eigenstate of σ_z corresponding to the larger eigenvalue. Then the initial statistical operator reads

$$\rho(0) = |+\rangle\langle+|\,. \tag{19}$$

We focus our attention on two aspects of heat conductance in flux qubits. The first is time evolution of the heat currents for different couplings presented in Fig. 1. We see that for short times, the heat currents are positive for an even number of electrons and are negative for an odd number of electrons. It is not a general rule: in dependence on coupling, the signs of

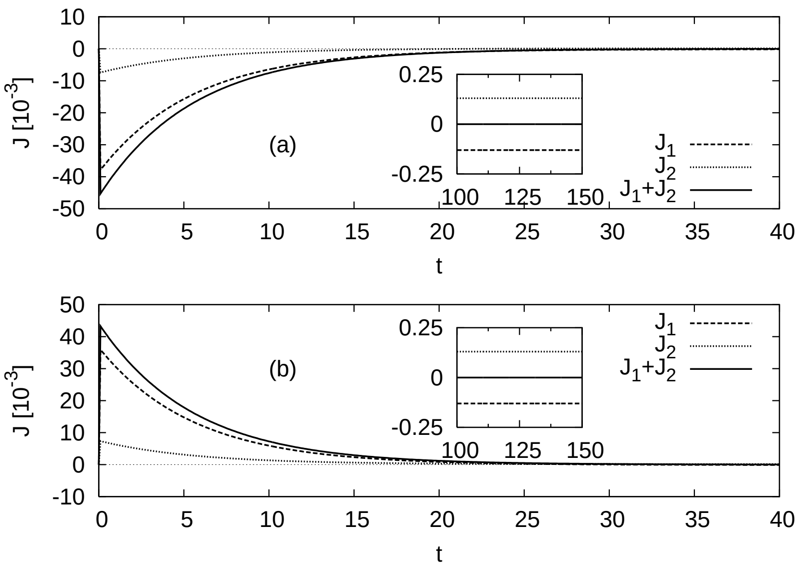

Fig. 1. Heat currents $J_1(t), J_2(t)$ and the total heat current $J(t)$ for the flux qubit coupled to two ohmic heat baths for the coupling $\sigma_x\sigma_z$: $w^{(1)} = 0, u^{(1)} = 1, w^{(2)} = 1, u^{(2)} = 0$ in Eq. (5). The temperatures of the heat baths are $T_1 = 10$ and $T_2 = 50$. The magnetic flux is fixed at $\phi/\phi_0 = 1/4$. The remaining parameters are: $\Delta = 1, B_x = 0.1, \alpha = 0.01, \omega_c = 100$. The panel (a) presents the heat current dynamics for the even number of electrons in the ring, while the panel (b) corresponds to the odd number of electrons. Note that the heat current $J_2(t)$ in the panel (a), being negative for short time, crosses the zero value at some time $t = t_p$ becoming positive for long time, *cf.* the inset therein. The change of sign of the heat current $J_1(t)$ occurs in the case depicted in the panel (b).

heat currents can be just opposite. Unfortunately, as the Davies theory for open systems is suitable mainly for long-time dynamics, the validity of this analysis is limited. From the numerical analysis one can present two main conclusions: the first is the $\sigma_x\sigma_z \leftrightarrow \sigma_z\sigma_x$ 'symmetry breaking' and the second that $\sigma_z\sigma_z$ coupling leads to the fastest saturation of the heat current to its steady-state value (not shown). The next aspect of heat conductance of non-superconducting flux qubits concerns 'controllability' of the heat flow by the externally applied magnetic flux which is related to the 'structural properties' of the qubits which can accommodate either even or odd number of electrons. The results are presented in Fig. 2. As the temperature enters non-linearly the system equations of motion, the linear dependence of the stationary heat current J_2 on the $(T_2 - T_1)$ difference is valid only in the classical limit [13]. Moreover, heat currents are highly ϕ-dependent as can be inferred form lower panels of Fig. 2. The most spectacular is a very small

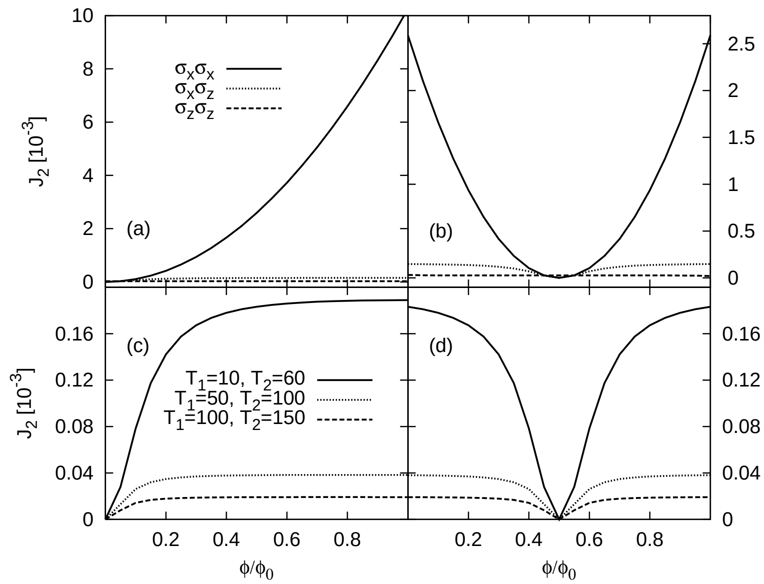

Fig. 2. Stationary heat current J_2 leaking through the flux qubit coupled to two ohmic baths controlled by the external magnetic flux ϕ/ϕ_0. Panels (a) and (c) correspond to an even number of electrons. Panels (b) and (d) correspond to an odd number of electrons. In panels (a) and (b), the temperatures of the heat baths are $T_1 = 10$ and $T_2 = 50$. These two panels (a) and (b) show the role of interaction between the qubit and reservoirs. The $\sigma_x\sigma_x$-coupling results in large stationary heat flow for the external magnetic flux $\phi/\phi_0 = 1$ (in panel (a)) or for $\phi/\phi_0 = 0$ and 1 (in panel (b)). In panels (c) and (d), the $\sigma_x\sigma_z$-coupling is assumed. Although the difference of temperatures is the same, $T_2 - T_1 = 50$, heat currents are different. It shows that the stationary current is not a linear function of the temperature difference. The remaining parameters are the same as in Fig. 1.

amplitude of the heat current J_2 for such magnetic fluxes ϕ that $B_z = 0$, see Eq. (2). This condition is satisfied either at $\phi/\phi_0 = 1/2$ for qubits built on mesorings accommodating an odd number of electrons or at $\phi/\phi_0 = 0$ for those built on mesorings accommodating an even number of electrons. This effect depends neither on the specific coupling to the baths (upper panels of Fig. 2) nor on temperatures (lower panels of Fig. 2).

5. Summary

Qubits based on the magnetic flux degree of freedom play a promising and important role in development of quantum information (maybe also for geometric or holonomic quantum computation [14]). Such systems may be less affected by uncontrolled fluctuations and therefore more robust against certain sources of perturbations. It is now known that solid-state qubits can provide decoherence times long enough to perform basic quantum algorithms. However, further increase of system complexity is facing the problem of heat and influence of surroundings of non-zero temperatures. There are cooling protocols in which a subset of qubits can be brought into contact with an external system of large heat capacity. The experimental realization of multi-step cooling of a quantum system via heat-bath algorithmic cooling has been performed [15]. Theoretical efforts to investigate transfer of heat in small systems can lead to implementation-independent cooling procedures. Quantum nanomachines and heat engines operate using quantum matter as their working substance [1]. The potential implementations of recently developed theoretical models require deep understanding of the thermodynamic properties of this 'substance'. In this paper we have chosen as 'the substance' the qubit based on non-superconducting mesoring. Such systems are not only smaller than the conventional superconducting rings as they do not operate in 'thermodynamic limit' required for superconductivity but also their properties can be controlled by adding or removing only a few electrons. Such a choice is motivated both by non-trivial properties of such systems in comparison with superconducting materials [5, 7] and by a natural need for finding alternative solutions for implementations based *e.g.* on carbon-made tubes, rings, belts or tori. We have shown that the heat transport in such systems weakly coupled to the environment exhibits various non-trivial properties which can be, relatively easily, controllable. It opens the possibility of applying non-superconducting qubits as a 'building blocks' for quantum thermodevices.

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