Quantum heat transport II
and
Hamiltonian in quantum circuit

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I. HEAT TRANSPORT BETWEEN ELECTRONS AND PHONONS

At low temperatures, phonons provide the heat bath to which electrons couple weakly in a mesoscopic electron circuit. Due to fast electron-electron relaxation, electrons typically obey Fermi-Dirac distribution even under non-equilibrium conditions with a well-defined temperature T_e that can differ from the temperature T_p of the phonons. A sketch of the system is schematically shown in Fig. 1(a). The normal metal is thermally coupled to the local phonon bath with thermal conductance $G_{\rm th}$ at temperature T_p. Applying power to the electron system, in practice normally by Joule heating, one creates temperature difference between the two subsystems. By measuring this difference, one can directly then deduce the heat current $\dot{Q}_{\rm ep}$ and thermal conductance $G_{\rm th}$ between electrons and phonons.

We make the following assumptions (adapted from [2]):

1. Uniform T of electrons, $T_e \ll T_F$, in fact $T_e/T_F \sim 10^{-6}$.

2. Phonons have a well-defined temperature $T_p \ll \theta_D$, the Debye temperature $\theta_D \sim 300$ K. Then only acoustic phonons with $\omega_q = c_l q$ exist.

3. We assume spherical Fermi surface for electrons.

4. We take coupling in metals to be represented by scaler deformation potential as to be discussed below.

5. Phonons are assumed to be 3D. This implies that the dimensions of the system are larger than the thermal wavelength, to be discussed in the lecture.

The total Hamiltonian describing the system and the environment is given by

$$H = H_e + H_p + H_{\rm ep}, \tag{1}$$

where H_e, H_p are the Hamiltonians of the electrons and phonons, respectively, and $H_{\rm ep}$ is the coupling between them (perturbation). The unperturbed Hamiltonian $H_0 = H_e + H_p$ can be written as

$$H_0 = \sum_k \epsilon_k a_k^\dagger a_k + \sum_q \hbar\omega_q c_q^\dagger c_q, \tag{2}$$

where the first part describes electron states with energy ϵ_k, momentum k, and $a_k^\dagger$ and a_k are the corresponding creation and annihilation operators, respectively. With analogous notation, the second part shows the Hamiltonian of phonons with eigenenergies $\hbar\omega_q$, wavevector q, and bosonic creation and annihilation operators $c_q^\dagger$ and c_q. The coupling term as a perturbation of the system has the following form in a metal (see Fig. 1(b))

$$H_{\rm ep} = \gamma \sum_{k,q} \omega_q^{1/2} (a_k^\dagger a_{k-q} c_q + a_k^\dagger a_{k+q} c_q^\dagger). \tag{3}$$

Here, the magnitude of γ (to be discussed later) depends on the material properties of the system. The operator of heat flux from the electron system to phonons due to electron-phonon coupling is

$$\dot{H}_p = \frac{i}{\hbar}[H_{\rm ep}, H_p] = i\gamma \sum_{k,q} \omega_q^{3/2} (a_k^\dagger a_{k-q} c_q - a_k^\dagger a_{k+q} c_q^\dagger), \tag{4}$$

where we used the commutation relations for the bosonic operators, $[c_q, c_q^\dagger c_q] = c_q$ and $[c_q^\dagger, c_q^\dagger c_q] = -c_q^\dagger$ and for fermions $\{a_k, a_k^\dagger\} = 1$.

Next, we apply the Kubo formula (that we explained in the note of the previous lecture) to obtain the ep heat flux $\dot{Q}_{\rm ep} = \langle \dot{H}_p \rangle$. Then we have

$$\langle \dot{H}_p \rangle = \langle \dot{H}_p \rangle_0 - \frac{i}{\hbar} \int_0^t dt' \langle [\dot{H}_p(t), H_{\rm ep}(t')] \rangle_0. \tag{5}$$

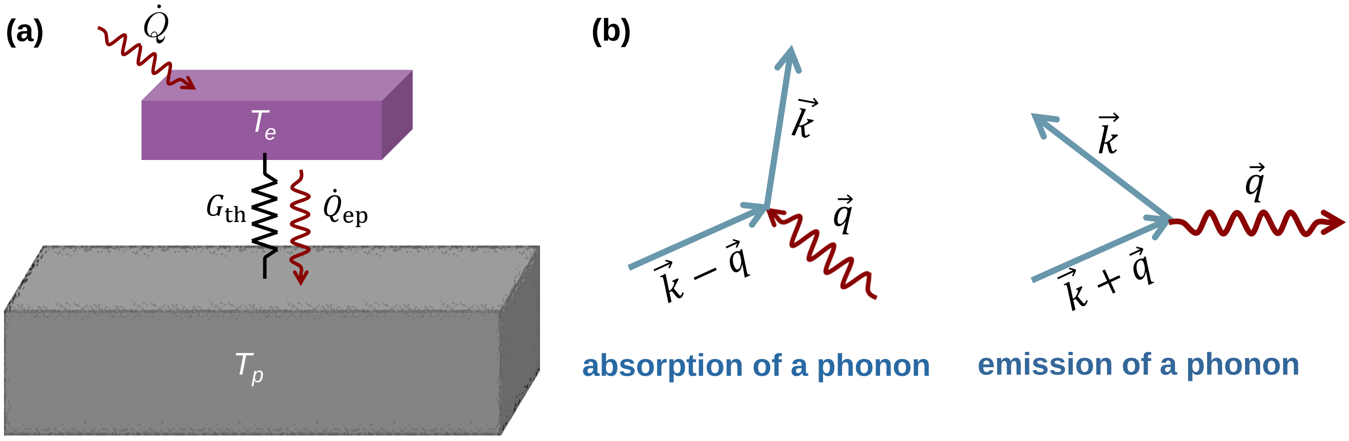

FIG. 1: (a) Normal metal with temperature T_e coupled to phonon bath (T_p) via electron-phonon coupling with heat current $\dot{Q}_{ep}$ and thermal conductance $G_{\rm th}$. (b) Emission and absorption of phonons of wave vector $\vec{q}$ and electron of wave vector $\vec{k}$.

The first $\langle \dot{H}_p \rangle_0 = 0$. For the second term we start by calculating the commutator

$$\begin{aligned}&[\dot{H}_p(t), H_{\rm ep}(t')] \\ &= [i\gamma \sum_{k,q} \omega_q^{3/2}(a_k^\dagger(t)a_{k-q}(t)c_q(t) - a_k^\dagger(t)a_{k+q}(t)c_q^\dagger(t)), \gamma \sum_{k',q'} \omega_{q'}^{1/2}(a_{k'}^\dagger(t')a_{k'-q'}(t')c_{q'}(t') + a_{k'}^\dagger(t')a_{k'+q'}(t')c_{q'}^\dagger(t'))].\end{aligned} \tag{6}$$

Here we have eight terms in the above equation. Take into account that the electrons and phonons are independent from each other meaning that they can commute and we neglect the double creation and double annihilation operators because they do not survive in the average. Therefore only four terms survive

$$\begin{aligned}[\dot{H}_p(t), H_{\rm ep}(t')] &= i\gamma^2 \sum_{k,q}\sum_{k',q'} \omega_q^{3/2}\omega_{q'}^{1/2} \\ &\Big(a_k^\dagger(t)a_{k-q}(t)c_q(t)a_{k'}^\dagger(t')a_{k'+q'}(t')c_{q'}^\dagger(t') - a_k^\dagger(t)a_{k+q}(t)c_q^\dagger(t)a_{k'}^\dagger(t')a_{k'-q'}(t')c_{q'}(t') \\ &+ a_{k'}^\dagger(t')a_{k'-q'}(t')c_{q'}(t')a_k^\dagger(t)a_{k+q}(t)c_q^\dagger(t) - a_{k'}^\dagger(t')a_{k'+q'}(t')c_{q'}^\dagger(t')a_k^\dagger(t)a_{k-q}(t)c_q(t)\Big).\end{aligned}$$

Next one needs to take the expectation values of the expressions in Eq. (7)

$$\langle a_k^\dagger(t)a_{k-q}(t)c_q(t)a_{k'}^\dagger(t')a_{k'+q'}(t')c_{q'}^\dagger(t')\rangle_0 = \langle a_k^\dagger(t)a_{k-q}(t)a_{k'}^\dagger(t')a_{k'+q'}(t')\rangle_0 \langle c_q(t)c_{q'}^\dagger(t')\rangle_0. \tag{7}$$

Here it is clear that $q = q'$. For the first part we use the "Wick's rule" for fermions the product of the creation and annihilation operator

$$\begin{aligned}\langle \hat{\Phi}|\hat{A}\hat{B}\hat{C}\hat{D}|\hat{\Phi}\rangle &= \langle \hat{\Phi}|\hat{A}\hat{B}|\hat{\Phi}\rangle\langle \hat{\Phi}|\hat{C}\hat{D}|\hat{\Phi}\rangle - \langle \hat{\Phi}|\hat{A}\hat{C}|\hat{\Phi}\rangle\langle \hat{\Phi}|\hat{B}\hat{D}|\hat{\Phi}\rangle + \\ &\langle \hat{\Phi}|\hat{A}\hat{D}|\hat{\Phi}\rangle\langle \hat{\Phi}|\hat{B}\hat{C}|\hat{\Phi}\rangle.\end{aligned} \tag{8}$$

Then for Eq. (7) we have

$$\begin{aligned}\langle a_k^\dagger(t)a_{k-q}(t)a_{k'}^\dagger(t')a_{k'+q}(t')\rangle_0 \langle c_q(t)c_q^\dagger(t')\rangle_0 &= \Big(\underline{\langle a_k^\dagger(t)a_{k-q}(t)\rangle_0} \langle a_{k'}^\dagger(t')a_{k'+q}(t')\rangle_0 - \underline{\langle a_k^\dagger(t)a_{k'}^\dagger(t')\rangle_0} \langle a_{k-q}(t)a_{k'+q}(t')\rangle_0 \\ &+ \langle a_k^\dagger(t)a_{k'+q}(t')\rangle_0 \langle a_{k-q}(t)a_{k'}^\dagger(t')\rangle_0 \Big) \langle c_q(t)c_q^\dagger(t')\rangle_0,\end{aligned} \tag{9}$$

where the two underlined terms are zero. For the third term we should have $k' = k - q$, which then becomes

$$\langle a_k^\dagger(t)a_{k-q}(t)a_{k'}^\dagger(t')a_{k'+q}(t')\rangle_0 \langle c_q(t)c_q^\dagger(t')\rangle_0 = \langle a_k^\dagger(t)a_k(t')\rangle_0 \langle a_{k-q}(t)a_{k-q}^\dagger(t')\rangle_0 \langle c_q(t)c_q^\dagger(t')\rangle_0 \tag{10}$$

$$= f(\epsilon_k)e^{i\epsilon_k(t-t')/\hbar}[1-f(\epsilon_{k-q})]e^{i\epsilon_{k-q}(t'-t)/\hbar}[1+n(\omega_q)]e^{i\omega_q(t'-t)}, \tag{11}$$

where $\langle c_q^\dagger(t)c_q(t)\rangle = n(\omega_q) = \frac{1}{e^{\beta\hbar\omega_q}-1}$ and $\langle c_q c_q(t)^\dagger(t)\rangle = 1+n(\omega_q)$is the Bose distribution for phonons. With the same procedure the rest of the terms in Eq. (7) reads

$$-\langle a_k^\dagger(t)a_{k+q}(t)a_{k'}^\dagger(t')a_{k'-q}(t')\rangle_0\langle c_q^\dagger(t)c_q(t')\rangle_0 = -f(\epsilon_k)[1-f(\epsilon_{k+q})]e^{i(\epsilon_{k+q}-\epsilon_k)(t'-t)/\hbar}n(\omega_q)e^{i\omega_q(t-t')} \tag{12}$$

$$\langle a_{k'}^\dagger(t')a_{k'-q'}(t')c_{q'}(t')a_k^\dagger(t)a_{k+q}(t)c_q^\dagger(t)\rangle_0 = f(\epsilon_{k+q})[1-f(\epsilon_k)]e^{i(\epsilon_{k+q}-\epsilon_k)(t'-t)/\hbar}[1+n(\omega_q)]e^{i\omega_q(t-t')} \tag{13}$$

$$-\langle a_{k'}^\dagger(t')a_{k'+q'}(t')c_{q'}^\dagger(t')a_k^\dagger(t)a_{k-q}(t)c_q(t)\rangle_0 = -f(\epsilon_{k-q})[1-f(\epsilon_k)]e^{i(\epsilon_{k-q}-\epsilon_k)(t'-t)/\hbar}n(\omega_q)e^{i\omega_q(t'-t)}. \tag{14}$$

By adding Eqs. (11)-(14) and shiffting the indices in Eq. (12), $k+q\to k$ and $k\to k-q$, and in Eq. (14) $k-q\to k$ and $k\to k+q$. We have

$$\begin{aligned}\langle[\dot{H}_p(t), H_{\rm ep}(t')]\rangle_0 \quad &= i\gamma^2\sum_{k,q}\omega_q^2\Big\{f(\epsilon_k)[1-f(\epsilon_{k-q})][1+n(\omega_q)](e^{i(\epsilon_{k-q}-\epsilon_k+\hbar\omega)(t'-t)/\hbar}+e^{-i(\epsilon_{k-q}-\epsilon_k+\hbar\omega)(t'-t)/\hbar})\\ &-f(\epsilon_k)[1-f(\epsilon_{k+q})]n(\omega_q)(e^{i(\epsilon_{k+q}-\epsilon_k-\hbar\omega)(t'-t)/\hbar}+e^{-i(\epsilon_{k+q}-\epsilon_k-\hbar\omega)(t'-t)/\hbar})\Big\}.\end{aligned} \tag{15}$$

Substituting Eq. (15) in (5), The electron-phonon heat flux reads

$$\dot{Q}_{\rm ep} = -\frac{i}{\hbar}\int_0^t dt'\langle[\dot{H}_p(t), H_{\rm ep}(t')]\rangle_0 \tag{16}$$

$$= 2\pi\gamma^2\sum_{k,q}\omega_q^2\Big\{f(\epsilon_k)[1-f(\epsilon_{k-q})][1+n(\omega_q)]\delta(\epsilon_{k-q}-\epsilon_k+\hbar\omega_q)-f(\epsilon_k)[1-f(\epsilon_{k+q})]n(\omega_q)\delta(\epsilon_{k+q}-\epsilon_k-\hbar\omega_q)\Big\} \tag{17}$$

$$\equiv \dot{Q}_{\rm emission}-\dot{Q}_{\rm absorption}, \tag{18}$$

where we used $\int_{-\infty}^0 dt'(e^{i\lambda t'}+e^{-i\lambda t'}) = \int_{-\infty}^\infty dt' e^{i\lambda t'} = 2\pi\delta(\lambda)$. We can first integrate over the angle θ between the electron and phonon wave vectors $\vec{k}$ and $\vec{q}$. Considering the 3D phonons in the spherical coordinates, we replace sum to

$$\sum_{k,q}\to\int_{-\infty}^\infty d\epsilon_k N(\epsilon_F)\int d^3q\mathcal{D}(q)\equiv\int_{-\infty}^\infty d\epsilon_k N(\epsilon_F)\Big\{\frac{\mathcal{V}}{(2\pi)^2}\int_0^\infty dq\, q^2\int_{-1}^1 d(\cos\theta)\Big\}, \tag{19}$$

where $\mathcal{D}(q) = \frac{\mathcal{V}}{(2\pi)^3}$ denotes the density of states of phonons with $\mathcal{V}$ as the volume of the system. Further, $\epsilon_k = \frac{\hbar^2k^2}{2m^*}$, $\epsilon_{k\pm q}\simeq\epsilon_k\pm\frac{\hbar^2k_F}{m^*}q\cos\theta$, where the last approximation is due to $k\simeq k_F$ and $q\ll k_F$. Here k_F is the Fermi wave vector of a spherical surface and m^* is the effective mass of electron in the metal in question. Next we replace ω_q with c_lq, where c_l is the velocity of sound in the normal metal. Substituting Eq. (19) into Eq. (17) we have

$$\begin{aligned}\dot{Q}_{\rm ep} = \quad &\frac{\gamma^2c_l^2N(\epsilon_F)\mathcal{V}}{2\pi}\int_{-\infty}^\infty d\epsilon_k\int_0^\infty dq\int_{-1}^1 d(\cos\theta)q^4\delta(\frac{\hbar^2k_F}{m^*}q\cos\theta-\hbar c_lq)\\ &\Big\{f(\epsilon_k)[1-f(\epsilon_k-\frac{\hbar^2k_F}{m^*}q\cos\theta)][1+n(\hbar c_lq)]-f(\epsilon_k-\frac{\hbar^2k_F}{m^*}q\cos\theta)[1-f(\epsilon_k)]n(\hbar c_lq)\Big\}.\end{aligned} \tag{20}$$

Collecting the angle dependent terms and integrating over $\cos\theta$ and using notation $\epsilon_q\equiv\hbar\omega_q = \hbar c_lq$, we have

$$\begin{aligned}\dot{Q}_{\rm ep} = \quad &\frac{\gamma^2c_l^2N(\epsilon_F)\mathcal{V}m^*}{2\pi\hbar^2k_F}\int_{-\infty}^\infty d\epsilon_k\int_0^\infty dq\ q^3\\ &\Big\{f(\epsilon_k)[1-f(\epsilon_k-\epsilon_q)][1+n(\epsilon_q)]-f(\epsilon_k-\epsilon_q)[1-f(\epsilon_k)]n(\epsilon_q)\Big\}.\end{aligned} \tag{21}$$

$$\begin{aligned}\dot{Q}_{\rm ep} = \frac{\gamma^2c_l^2N(\epsilon_F)\mathcal{V}m^*}{2\pi\hbar^2k_F} \quad &\Big\{\int_{-\infty}^\infty d\epsilon_k\int_0^\infty dq\ q^3f(\epsilon_k)[1-f(\epsilon_k-\epsilon_q)]\\ &+\int_{-\infty}^\infty d\epsilon_k\int_0^\infty dq\ q^3[f(\epsilon_k)-f(\epsilon_k-\epsilon_q)]n(\epsilon_q)\Big\}.\end{aligned} \tag{22}$$

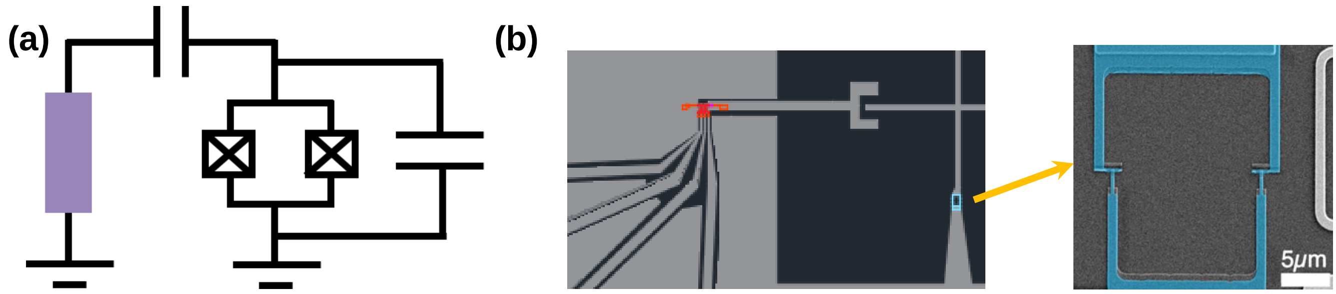

FIG. 2: Exemplary quantum circuit for analysis. (a) Circuit diagram. On the right side a SQUID (superconducting quantum interference device) composed of two Josephson junctions. This element is capacitively coupled to a resistive element on the left. (b) The actual on-chip circuit. The coupling capacitor is the fork-like structure in the middle, and the SQUID is zoomed out in blue on the right. The resistive element is contacted by four NIS tunnel junctions to control and measure temperature, on the left.

Calculating the integral over energies first, we have

$$\begin{aligned}\dot{Q}_{\text{ep}} = \; & \frac{\gamma^2 c_l^2 N(\epsilon_F)\mathcal{V}m^*}{2\pi\hbar^2 k_F}\left\{\int_0^\infty dq\; q^3 \frac{\epsilon_q}{e^{\beta_e \epsilon_q}-1} - \int_0^\infty dq\; q^3\; n(\epsilon_q)\; \epsilon_q\right\} \\ & \frac{\gamma^2 c_l^3 N(\epsilon_F)\mathcal{V}m^*}{2\pi\hbar k_F}\left\{\int_0^\infty dq\; q^4\left(\frac{1}{e^{\beta_e\hbar c_l q}-1} - \frac{1}{e^{\beta_p \hbar c_l q}-1}\right)\right\}.\end{aligned} \tag{23}$$

Considering $\int_0^\infty dx \frac{x^4}{e^{\beta x}-1} = \frac{24\zeta(5)}{\beta^5}$, where $\zeta(z)$ denotes the Riemann zeta function, we have

$$\dot{Q}_{\text{ep}} = \Sigma\mathcal{V}(T_e^5 - T_p^5), \tag{24}$$

where $\Sigma = \frac{12\gamma^2 N(\epsilon_F)m^*\zeta(5)k_B^5}{\pi k_F c_l^2 \hbar^6}$ is the electron-phonon coupling constant. Since for a metal with density ρ, $\gamma^2 = \frac{k_F^5\hbar^3}{36\pi^2 c_l^2 N(\epsilon_F)m^*\rho}$, we have

$$\Sigma = \frac{\zeta(5)k_B^5 k_F^4}{3\pi^3 c_l^4 \hbar^3 \rho}. \tag{25}$$

II. SUPERCONDUCTING QUANTUM CIRCUITS

We want to analyze eventually the circuit which is shown in Fig. 2(a). How do we see it? The qubit on the right side of Fig. 2(a) (coloured blue in Fig. 2(b)) is (almost) a two-level system that is influencedby the coupling to the noise source on the left. The later induces transitions in the qubit such that the steady-state population of the qubit is as in Lecture-1:

$$\rho_{ee} = 1 - \rho_{gg} = \frac{1}{1+e^{\beta\hbar\omega}}. \tag{26}$$

Instead of qubit we start with an LC-oscillator, shown in Fig. 3(a), and write its Hamiltonian

$$T = \frac{1}{2}C\dot{\Phi}^2 \tag{27}$$

$$V = \frac{\Phi^2}{2L}, \tag{28}$$

where $\Phi = \int_0^t dt'\; v(t')$ with v as voltage. The Lagrangian of the circuit is then

$$\mathcal{L} = T - V = \frac{1}{2}C\dot{\Phi}^2 - \frac{\Phi^2}{2L}, \tag{29}$$

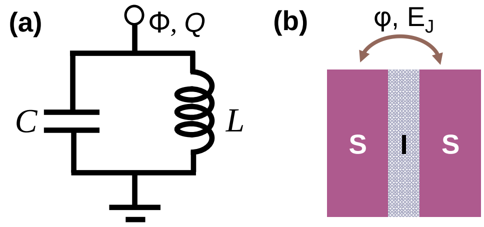

FIG. 3: (a) LC circuit. (b) Josephson junction.

From the Lagrangian we can obtain the conjugate momenta of node flux by the Legendre transformation

$$Q = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}} = C\dot{\Phi}, \tag{30}$$

where Q is the charge on the capacitor. Then we have

$$H = T + V = \frac{Q^2}{2C} + \frac{\Phi^2}{2L}. \tag{31}$$

Introducing the creation and annihilation operators such that

$$[c, c^\dagger] = 1, \tag{32}$$

we have

$$\Phi = \sqrt{\frac{\hbar Z_0}{2}}(c + c^\dagger) \tag{33}$$

$$Q = -i\sqrt{\frac{\hbar}{2Z_0}}(c - c^\dagger) \tag{34}$$

$$H = \frac{\hbar\omega_0}{2}(c^\dagger c + cc^\dagger) = \hbar\omega_0(c^\dagger c + \frac{1}{2}), \tag{35}$$

where $\omega_0 = \sqrt{\frac{1}{LC}}$, and $Z_0 = \sqrt{\frac{L}{C}}$. For a Josephson tunnel junction, shown in Fig. 3(b), the Josephson relations are

$$\hbar\dot{\phi} = 2ev \tag{36}$$

$$I = I_c \sin\phi, \tag{37}$$

where ϕ is the phase difference across the junction and v is the voltage. The first relation implies that flux and phase are related by

$$\phi = \frac{2e}{\hbar}\Phi. \tag{38}$$

In the second Josephson relation, I is the current through the junction and the r.h.s. applies for a tunnel junction, with critical current I_c. for different types of weak links, sinusoidal dependence does not necessarily hold. We discussed earlier that energy stored in the system (=work done by the source) is

$$E = \int^t Iv(t')dt' = I\Phi. \tag{39}$$

Thus for a current biased case $I = \frac{\partial E}{\partial \Phi}$ and

$$E = \int^\Phi I \, d\Phi \quad = \frac{\hbar I_c}{2e}\int^\phi \sin\phi' d\phi' \tag{40}$$

$$= -\frac{\hbar I_c}{2e}\cos\phi \equiv -E_J \cos\phi. \tag{41}$$

We call this Josephson energy and in quantum mechanics Josephson Hamiltonian $\hat{H}_J$. Now we may expand this energy for small values of ϕ, as

$$E \simeq -E_J(1-\frac{\phi^2}{2}) = \frac{E_J}{2}\phi^2 = (\frac{2e}{\hbar})^2\Phi^2 \equiv \frac{\Phi^2}{2L_J}. \tag{42}$$

Here $L_J = (\frac{\hbar}{2e})^2\frac{1}{E_J} = \frac{\hbar}{2eI_c}$ is the Josephson inductance. Therefore, in the linear regime:

$$\hat{H} = \frac{\hat{Q}^2}{2C} + \frac{\hat{\Phi}^2}{2L_J}, \tag{43}$$

i.e. Josephson junction behaves approximately as a harmonic oscillator.

Problem 5.1: On the lecture, we wrote the operator $\dot{H}_p$ for the heat current to the phonons (Eq. (4)). Write the corresponding operator for heat current to electrons $\dot{H}_e$, and show that assuming microscopic energy conservation, $\epsilon_k - \epsilon_{k-q} = \hbar\omega_q$, $\dot{H}_e = -\dot{H}_p$ **(1.5 points)**

Problem 5.2: Consider a classical Josephson junction where you ignore the charging energy $\frac{Q^2}{2C}$. Apply bias current to it. Show that the energy as a function of phase forms a washboard potential. According to the first Josephson relation show and argue that the critical current of the junction (i.e. the maximum sustainable supercurrent)$=\frac{2e}{\hbar}E_J$. **(1.5 points)**

The deadline for Problems 5.1 and 5.2 (3 points) is on Monday November 16 at noon, before the lecture.

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[1] Jukka P. Pekola and Bayan Karimi, Quantum noise of electron-phonon heat current, J. Low Temp. Phys. **191**, 373 (2018).
[2] F. C. Wellstood, C. Urbina, and John Clarke, Hot-electron effects in metals, Phys. Rev. B **49**, 5942 (1994).