Introduction to Chapter 6 (from Chapter 3 of the lecture notes)

Quantum treatment of JJ

3.6 Full Quantum Treatment of Josephson Junctions Secondary Quantum Macroscopic Effects

Classical treatment of Josephson junctions (so far)

Phase φ and charge $Q = CV \propto \frac{d\varphi}{dt}$ \rightarrow Purely classical variables (Q, φ) are assumed to be measurable simultaneously Dynamics \rightarrow Tilted washboard potential, rotating pendulum Classical energies:

→ Potential energy $U(\varphi)$

(Josephson coupling energy / Josephson inductance)

ightarrow Kinetic energy $K(\dot{\varphi})$

(Charging energy via $\frac{1}{2}CV^2 = \frac{Q^2}{2C} \propto \left(\frac{d\varphi}{dt}\right)^2$ / junction capacitance)

Current-phase & voltage-phase relation from macroscopic quantum model

- \rightarrow Quantum origin
- ightarrow Primary macroscopic quantum effects

Second quantization

- \rightarrow Treat (Q, φ) as quantum variables (commutation relations, uncertainty)
- \rightarrow Secondary macroscopic quantum effects



-> Classical treatment valid for $\frac{E_{J0}}{\hbar\omega_p} \simeq \left(\frac{E_{J0}}{E_C}\right)^{1/2} \gg 1$ (Level spacing \ll Potential depth)

 $E_C \propto 1/C \propto 1/A$ $E_{J0} \propto I_c \propto A$

 \rightarrow Enter quantum regime by decreasing junction area A

Parameters for the quantum regime

Example 1 Area $A = 10 \ \mu m^2$, Tunnel barrier d = 1 nm, $\varepsilon = 10$, $J_{\rm c} = 100 \frac{\rm A}{\rm cm^2}$ $\rightarrow E_{I0} = 3 \times 10^{-21} \text{ J}$ $\rightarrow E_{\text{I0}}/h = 4500 \text{ GHz}$ $C = \frac{\varepsilon \varepsilon_0 A}{d} = 0.9 \text{ pF}$ $\rightarrow E_C = 2 \times 10^{-26} \text{ J}$ $\rightarrow \frac{E_C}{h} = 30 \text{ MHz}$ \rightarrow Classical junction





 \rightarrow We also need $T \ll 500$ mK for $k_{\rm B}T \ll E_{\rm I0}$, $E_C!$

Hamiltonian of a strongly underdamped junction (with $\frac{d\varphi}{dt} \neq 0$) Kinetic energy: $K = \frac{1}{2}CV^2 = \frac{Q^2}{2C} = \frac{1}{2}C\left(\frac{\hbar}{2e}\right)^2\dot{\varphi}^2 = \frac{1}{2}E_{J0}\frac{\dot{\varphi}^2}{\omega_p^2}$

 \rightarrow Energy due to extra charge Q on one junction electrode due to V

Total energy:
$$E = K + U = E_{J0} \left(1 - \cos \varphi + rac{1}{2} rac{\dot{\varphi}^2}{\omega_p^2}
ight)$$

 $U(\varphi) \propto 1 - \cos \varphi \quad \rightarrow$ Potential energy $K(\dot{\varphi}) \propto \dot{\varphi}^2 \quad \rightarrow$ Kinetic energy

Consider $E(\varphi, \dot{\varphi})$ as junction Hamiltonian, rewrite kinetic energy

$$K = \frac{Q^2}{2C} = \frac{1}{2} \underbrace{\frac{1}{(\hbar/2e)^2 C}}_{1/\text{mass}} \underbrace{\left(\frac{\hbar}{2e}Q\right)^2}_{\text{momentum}} \qquad K = \frac{p^2}{2M} \rightarrow p = \left(\frac{\hbar}{2e}\right)Q$$

 \rightarrow Position coordinate associated to phase φ , momentum associated to charge Q



Hamiltonian in the flux basis (
$$\phi = \frac{\hbar}{2e} \varphi = \frac{\Phi_0}{2\pi} \varphi$$
)

$$\mathcal{H} = \frac{Q^2}{2C} + E_{J0} \left(1 - \cos 2\pi \frac{\phi}{\Phi_0} \right) = -\frac{(2e)^2}{2C} \frac{\hbar^2}{(2e)^2} \frac{\partial^2}{\partial \phi^2} + E_{J0} \left(1 - \cos 2\pi \frac{\phi}{\Phi_0} \right)$$
$$= -\frac{\hbar^2}{2C} \frac{\partial^2}{\partial \phi^2} + E_{J0} \left(1 - \cos 2\pi \frac{\phi}{\Phi_0} \right)$$

Commutator $[\phi, Q] = i\hbar$

- $\rightarrow \phi$ and Q are canonically conjugate (analogous to x and p)
- ightarrow Circuit variables are now quantized
- \rightarrow Superconducting quantum circuits

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The phase regime

 $\hbar \omega_{\rm p} \ll E_{\rm J0}$, $E_C \ll E_{\rm J0} \rightarrow$ Phase φ is a good quantum number!

Lowest energy levels localized near bottom of potential wells at $\varphi_n=2\pi~n$

Taylor series for $U(\varphi) \rightarrow$ Harmonic oscillator,

Frequency $\omega_{\rm p}$, eigenenergies $E_n = \hbar \omega_{\rm p} \left(n + \frac{1}{2} \right)$

Ground state: narrowly peaked wave function at $\varphi = \varphi_n$

Large fluctuations of Q on electrodes since $\Delta Q \cdot \Delta \phi \ge 2e$ (small $E_c \rightarrow$ pairs can easily fluctuate, large ΔQ)

Small phase fluctuations $\Delta \varphi$

Negligible $\Delta \phi \Rightarrow$ classical treatment of phase dynamics is good approximation

3.6.2 Limiting Cases: The Phase and Charge Regime

The phase regime

Hamiltonian

$$H = -4E_C \frac{\partial^2}{\partial \varphi^2} + E_{J0}(1 - \cos \varphi)$$

define
$$a = (E - E_{J0})/E_C$$
, $b = E_{J0}/2E_C$ and $z = \varphi/2$

→ Mathieu equation
$$\frac{\partial^2 \Psi}{\partial z^2} + (a + 2b\cos 2z)\Psi = 0$$

known from periodic potential problem in solid state physics → Energy bands

General solution

Bloch waves

$$\psi_q(\varphi) = u_q(\varphi) \exp(\imath q \varphi)$$
 with $u_q(\varphi) = u_q(\varphi + 2\pi)$

Charge/pair number variable q is continuous (charge on capacitor!) $\rightarrow \Psi(\varphi)$ is not 2π -periodic

 $\Psi(\varphi) = \sum_{a} c_q \psi_q$

3.6.2 Limiting Cases: The Phase and Charge Regime

The phase regime

1D problem → Numerical solution straightforward Variational approach for **approximate** ground state

Trial function for
$$E_C \ll E_{\text{J0}} \quad \Psi(\varphi) \propto \exp\left(-\frac{\varphi^2}{4\sigma^2}\right)$$

Choose σ to find minimum energy:



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The phase regime

Tunneling coupling $\propto \exp\left(-\frac{2E_{J0}-E}{\hbar\omega_p}\right)$ > Very small since $\hbar\omega_p \ll E_{J0}$ > Tunneling splitting of low lying states is exponentially small

$$E_{\min} = E_{J0} \left(1 - \left[1 - \sqrt{\frac{2E_C}{E_{J0}}} \right]^2 \right) = E_{J0} \left(1 - \left[1 - \frac{\hbar\omega_p}{2E_{J0}} \right]^2 \right)$$



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The charge regime

 $\hbar\omega_{\rm p} \gg E_{\rm J0}$, $E_C \gg E_{\rm J0} \rightarrow$ Charge Q (momentum) is good quantum number

Kinetic energy $\propto E_c \left(\frac{d\varphi}{dt}\right)^2$ dominates

- \rightarrow Complete delocalization of phase
- → Wave function should approach constant value, $\Psi(\varphi) \simeq \text{const.}$
- → Large phase fluctuations, small charge fluctuations ($\Delta Q \cdot \Delta \phi \geq 2e$)

Hamiltonian

$$\mathcal{H} = -4E_C \frac{\partial^2}{\partial \varphi^2} + E_{J0}(1 - \cos \varphi)$$

Appropriate trial function: $\Psi(arphi) \propto (1 - lpha \cos arphi)$ $lpha \ll 1$

Approximate ground state energy

$$E_{\min} \simeq E_{J0} \left(1 - \frac{E_{J0}}{8E_C} \right) = E_{J0} \left(1 - \frac{E_{J0}^2}{(\hbar\omega_p)^2} \right)$$

second order in E_{J0}

3.6.2 Limiting Cases: The Phase and Charge Regime

The charge regime





ightarrow Periodic potential is weak

- \rightarrow Strong coupling between neighboring phase states \rightarrow Broad bands
- → Compare to electrons moving in strong (phase regime) or weak (charge regime) periodic potential of a crystal

Coulomb blockade in normal metal tunnel junctions

Voltage
$$V \rightarrow$$
 Charge $Q = CV$, energy $E = \frac{Q^2}{2C}$

Single electron tunneling

- \rightarrow Charge on one electrode changes to Q e
- → Electrostatic energy $E' = \frac{(Q-e)^2}{2C}$
- → Tunneling only allowed for $E^{i} \leq E$
- → Coulomb blockade: Need $|Q| \ge e/2$ or $|V| \ge V_{CB} = V_c = e/2C$

Observation of CB requires small thermal fluctuations

$$\Rightarrow E_C = \frac{e^2}{2C} > k_B T \Rightarrow C < \frac{e^2}{2k_B T}$$

$$\Rightarrow C \simeq 1 \text{ fF at } T = 1 \text{ K}, d = 1 \text{ nm, and } \varepsilon = 5 \Rightarrow A \leq 0.02 \text{ } \mu\text{m}^2 \Rightarrow \text{Small junctions!}$$

Observation of CB requires small quantum fluctuations

 \rightarrow Quantum fluctuations due to Heisenberg principle $\rightarrow \Delta E \cdot \Delta t \geq \hbar$

ightarrow Finite tunnel resistance

 $\rightarrow \tau_{RC} = RC$ (decay of charge fluctuations)

$$\rightarrow \Delta t = 2\pi RC, \ \Delta E = \frac{e^2}{2C} \rightarrow R \ge \frac{h}{e^2} = R_K = 24.6 \text{ k}\Omega \rightarrow \text{Typically satisfied}$$



Coulomb blockade in superconducting tunnel junctions V R_s R, C

For $\frac{Q^2}{2C} > k_B T$, eV $(Q = 2e) \rightarrow \text{No flow of Cooper pairs}$ Threshold voltage $\rightarrow |V| \ge V_{CB} = V_c = \frac{2e}{2C} = \frac{e}{C}$

Coulomb blockade \rightarrow Charge is fixed, phase is completely delocalized

3.6.3 Coulomb and Flux Blockade

Phase or flux blockade in a Josephson junction

Current $I \rightarrow$ Flux $\Phi = L I$, energy $E = \Phi^2/2L$

→ Phase is blocked due to large $E_{J0} = \Phi_0 I_c / 2\pi$

 $\rightarrow I_{\rm c}$ takes the role of $V_{\rm CB}$

 \rightarrow Phase change of 2π equivalent to flux change of Φ_0

→ Flux blockade $|I| \ge I_{FB} = I_c = \frac{(\Phi_0/2\pi)}{L_c}$

$$\rightarrow$$
 Analogy to CB $\rightarrow I \leftrightarrow V$, $2e \leftrightarrow \frac{\Phi_0}{2\pi}$, $C \leftrightarrow L$

$$L_c = \frac{\hbar}{2eI_c}$$

s

R_s

S

R, L

In presence of fluctuations we need $\Rightarrow E_{J0} \gg k_B T$ (large junction area) $\Rightarrow \text{And } \Delta E \cdot \Delta t \ge \hbar \text{ with } \Delta t = 2\pi \frac{L}{R} \text{ and } \Delta E = 2E_{J0} \Rightarrow R \le \frac{h}{(2e)^2} = \frac{1}{4}R_K$

3.6.4 Coherent Charge and Phase States

Coherent charge states Island charge continuously changed by gate Ε Q²/2C EJO Ē Emin 2 3 Q/2e 0



Cooper pair box

Independent charge states ($E_{J0} = 0$) → Parabola $E(Q) = (Q - n \cdot 2e)^2/2C_{\Sigma}$

 $E_{\rm J0} > 0$

→ Interaction of $|n\rangle$ and $|n + 1\rangle$ at the level crossing points $Q = \left(n + \frac{1}{2}\right) \cdot 2e$

- → Avoided level crossing (anti-crossing)
- → Coherent superposition states $|\Psi_{\pm}\rangle = \alpha |n\rangle \pm \beta |n+1\rangle$

Coherent charge states

Average charge on the island as a function of the applied gate voltage \rightarrow Quantized in units of 2*e* (no coherence yet)



First experimental demonstration of coherent superposition charge states by Nakamura, Pashkin, Tsai (1999, not this picture)

3.6.4 Coherent Charge and Phase States



Tunnel coupling $\rightarrow \quad \Psi_{\pm} = a|L\rangle \pm b|R\rangle$ Experimental evidence for quantum coherent superposition (Mooij et al., 1999)

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Violation of conservation of energy on small time scales, obey $\Delta E \cdot \Delta t \geq \hbar$

- → Creation of **virtual excitations**
- \rightarrow Include Langevin force I_F with adequate statistical properties
- \rightarrow Fluctuation-dissipation theorem

$$S_{I}(f) = 2\pi S_{I}(\omega) = 4 \frac{E(\omega, T)}{R_{N}} \qquad E(\omega, T) = \text{energy of a quantum oscillator}$$

$$E(\omega, T) = \frac{\hbar\omega}{2} + \hbar\omega \frac{1}{\exp\left(\frac{\hbar\omega}{k_{B}T}\right) - 1} = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_{B}T}\right)$$
vacuum occupation probability of oscillator (Planck distribution)

→ Transition from "thermal" Johnson-Nyquist noise to quantum noise:

classical limit (
$$\hbar\omega$$
, $eV \ll k_BT$): $S_I(\omega) = \frac{1}{2\pi} \frac{4k_BT}{R_N}$

quantum limit (
$$\hbar\omega, eV \gg k_BT$$
): $S_I(\omega) = \frac{1}{2\pi} \frac{2\hbar\omega}{R_N} = \frac{1}{2\pi} \frac{2eV}{R_N}$

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3.6.6 Macroscopic Quantum Tunneling

Escape of the "phase particle" from minimum of washboard potential by tunneling

→ Macroscopic, i.e., phase difference is tunneling (collective state)

→ States easily distinguishable

Competing process

- → Thermal activation
- \rightarrow Low temperatures

Neglect damping Dc-bias \rightarrow Term $-\frac{\hbar I \varphi}{2e}$ in Hamiltonian

Curvature at potential minimum:

$$\frac{\partial^2 U}{\partial \varphi^2} = E_{J0} \sqrt{1 - i^2} \qquad i = I/I_c$$

(Classical) small oscillation frequency:

$$\omega_{\mathcal{A}} = \omega_p (1 - i^2)^{1/4}$$
 (attempt frequency)



Quantum mechanical treatment

 \rightarrow Tunnel coupling of bound states to outgoing waves \rightarrow Continuum of states

- \rightarrow But only states corresponding to quasi-bound states have high amplitude
- \rightarrow In-well states of width $\Gamma = \hbar/\tau$ ($\tau =$ lifetime for escape)

Determination of wave functions

 \rightarrow Wave matching method

→ Exponential prefactor within WKB approximation

 \rightarrow Decay in barrier:

$$|\Psi(x)|^2 \propto \exp\left\{-\frac{2}{\hbar}\int\limits_{||}\sqrt{2M[V(x)-E]}\ dx
ight\}$$

decay of wave function of particle with mass M and energy E

for
$$U(\varphi) \gg E_0 = \hbar \omega_A/2$$

 $|\Psi(\varphi)|^2 \propto \exp\left\{-\frac{2}{\hbar} \int_{||} \sqrt{2\left(\frac{\hbar}{2e}\right)^2 C\left[U(\varphi) - \frac{\hbar \omega_A}{2}\right]} d\varphi\right\}$
mass effective barrier height

3.6.6 Macroscopic Quantum Tunneling

Constant barrier height
$$\Rightarrow$$
 Escape rate $|\Psi(\varphi)|^2 \propto \exp\left\{-\frac{2}{h}\int_{\Pi} \sqrt{2\left(\frac{h}{2e}\right)^2 c\left[U(\varphi) - \frac{h\omega_A}{2}\right]} d\varphi\right\}$
 $|\Psi(\varphi)|^2 \propto \exp\left\{-\sqrt{\frac{U_0}{E_C}} \Delta\varphi\right\} \Rightarrow \Gamma = \frac{\omega_A}{2\pi} \exp\left\{-\sqrt{\frac{U_0}{E_C}} \Delta\varphi\right\}$
Increasing bias current \Rightarrow
 $U_0 \simeq 2E_{J0}(1-i^2)^{3/2}$ and $\Delta\varphi \simeq \pi \sqrt{1-i^2}$
 U_0 decreases with $i \Rightarrow \Gamma$ becomes measurable
Temperature T^* where $\Gamma_{\text{tunnel}} = \Gamma_{\text{TA}} \approx \exp\left(-\frac{U_0}{k_BT}\right)$
for $I \simeq 0$: $U_0 \simeq 2E_{J0}$ $\hbar\omega_p = \sqrt{8E_{J0}E_C} \simeq 2\sqrt{U_0E_C}$ $\Delta\varphi \simeq \pi$
 $\Rightarrow \Gamma = \frac{\omega_p}{2\pi} \exp\left\{-2\pi \frac{U_0}{\hbar\omega_p}\right\} \Rightarrow k_B T^* \simeq \frac{\hbar\omega_p}{2\pi}$
for $I > 0$: $\sqrt{U_0} \propto (1-i^2)^{3/4}$ $\Delta\varphi \propto (1-i^2)^{1/2}$
 $\Rightarrow k_B T^* \simeq \frac{\hbar\omega_A}{2\pi} = \frac{\hbar\omega_p}{2\pi}(1-i^2)^{1/4}$
For $\omega_p \approx 10^{11} s^{-1}$

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Additional topic: Effect of damping

Junction couples to the environment (e.g., Caldeira-Leggett-type heat bath)

→ Crossover temperature $k_B T^* \approx \frac{\hbar \omega_R}{2\pi}$ with $\omega_R = \omega_A (\sqrt{1 + \alpha^2} - \alpha)$ and $\alpha \equiv \frac{1}{2R_N C \omega_A}$ → Strong damping $\alpha \gg 1 \rightarrow \omega_{\rm R} \ll \omega_{\rm A} \rightarrow$ Lower T^{\star} → Damping suppresses MQT 1.0 0.8 10^{3} $\omega_{
m R}/\omega_{
m A}$ 0.6 0.4 lightly damped (small capacitance) 0.2 "quantum junction" T_{esc} (mK) I. = 9.489 µA 0 10² 10^{-3} 10^{-1} 10^{3} 10^{5} 10 α "classical junction" Ic = 1.383 µA Phase diffusion by MQT moderately damped (larger capacitance) See lecture notes 10¹ 10² 10^{3} 10 T (mK)

After: Martinis *et al.*, Phys. Rev. B. **35**, 4682 (1987).

Summary (secondary quantum macroscopic effects)

Classical description only in the phase regime (large junctions): $E_C \ll E_{J0}$

For $E_c \gg E_{J0}$: quantum description (negligible damping):

$$\mathcal{H} = 4E_C \frac{\partial^2}{\partial \varphi^2} + E_{J0}(1 - \cos \varphi)$$

Phase difference φ and Cooper pair number $N = \frac{Q}{2\rho}$ are canonically conjugate variables

$$[\varphi, \frac{h}{2e}Q] = i\hbar \qquad \Rightarrow \Delta N \cdot \Delta \varphi \ge 1$$

phase regime: $\Delta \varphi \rightarrow 0$ and $\Delta N \rightarrow \infty$ charge regime: $\Delta N \rightarrow 0$ and $\Delta \varphi \rightarrow \infty$

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Charge regime at T = 0
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→ Coulomb blockade → Tunneling only for $V_{CB} \ge \frac{e}{c}$ Flux regime at T = 0

→ Flux blockade → Flux motion only for $I_{\text{FB}} \ge \frac{\Phi_0}{2\pi L_c}$

At $I < I_c$

 \rightarrow Escape out of the washboard by thermal activation or macroscopic quantum tunneling

TA-MQT crossover temperature T^{\star}

$$k_B T^* \simeq \frac{\hbar \omega_A}{2\pi} = \frac{\hbar \omega_p}{2\pi} \left[1 - \left(\frac{l}{l_c}\right)^2 \right]^{1/4}$$