Homework assignment 4 - Superconductivity and the basics of superconducting qubits

Semiconducting & Superconducting Quantum Computers

Due: Nov 6th, 2022

Problem 1 - Flux quantization and gauge transformation (15 pts / no collaboration)

In the superconducting state of a metal, the electrons close to the Fermi energy pair up with opposite spins and momenta to form Cooper pairs. In this condensate, all the Cooper pairs will have the same energy and they realize a macroscopic quantum state across the entire piece of the superconductor. Because this superconducting condensate is a coherent quantum state, it can be described by a wavefunction, which takes the form of

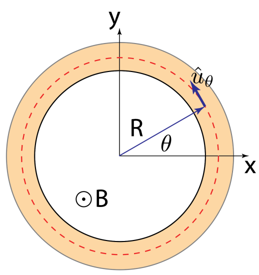
$$\psi(\mathbf{r}) = \sqrt{n_s/2}e^{i\varphi(\mathbf{r})}, \tag{1}$$

where $\mathbf{r}$ is the position inside the superconductor, n_s is the density of the superconducting Cooper pairs and $\varphi(\mathbf{r})$ is the phase of the wavefunction. While inside the superconductor the amplitude of the wavefunction $\sqrt{n_s/2}$ is constant, the phase $\varphi(\mathbf{r})$ can change as a function of position. In this problem, we investigate how the phase behaves in a cylindrical superconductor in magnetic field.

a) We discussed in class that inside the superconductor, where the magnetic field is zero $\mathbf{B} = 0$, the supercurrent vanishes, and the phase is directly related to the vector potential $\mathbf{A}$ such that

$$\mathbf{A} = \frac{\Phi_0}{2\pi}\nabla\varphi, \tag{2}$$

where $\Phi_0 = h/2e$ is the flux quantum. We consider a thin cylindrical superconductor with radius R and long axis oriented along the z direction (see Figure below). The external magnetic field also points along the z axis, and has magnitude of B_0 such that $\mathbf{B} = (0, 0, B_0)$ in the Cartesian $x - y - z$ coordinate system. Importantly, the choice of the vector potential $\mathbf{A}$ is not unique; as long as it satisfies that $\mathbf{B} = \nabla \times \mathbf{A}$, the vector potential describes correctly the system. Consequently, the phase of the superconductor is neither unique, which is not surprising given that the phase of a wavefunction is not an observable quantity.



We are interested to solve how the phase evolves inside the superconductor as a function of the angle θ, where θ is measured relative to the x axis. First, we consider the Coulomb gauge, i.e. $\nabla\mathbf{A} = 0$, so that $\mathbf{A} = (-yB_0/2, xB_0/2, 0)$. Show that this choice of the vector potential is correct because $\mathbf{B} = \nabla \times \mathbf{A}$. By integrating Eq. (2) and assuming that the phase reference is such that $\varphi(\theta = 0) = 0$, determine the phase of the superconducting wavefunction as function of the angle θ,

$$\varphi(\theta) = \int_0^\theta \frac{2\pi}{\Phi_0}\mathbf{A}\hat{u}_\theta R d\theta, \tag{3}$$

where $\hat{u}_\theta = (-\sin\theta, \cos\theta, 0)$ is the unit vector along the integration path (see Figure). Show that because the phase needs to be 2π periodic, the enclosed flux in the cylinder needs to be an n integer multiple of the flux quantum $\Phi = n\Phi_0$. Plot the phase of the wavefunction as a function of the angle $\varphi(\theta)$ for the case of $n = 0, 1, 2, 3$.

b) Calculate the superconducting phase $\varphi'(\theta)$ for the case of another valid choice of the vector potential $\mathbf{A}' = (0, xB_0, 0)$, and plot it in case the number of enclosed flux quantum is $n = 0, 1, 2, 3$.

c) Although the two different vector potentials lead to two different phase behavior, they are connected by a quantum gauge transformation. Generally, it can be shown that if the vector potential is changed by a transformation such that

$$\mathbf{A}' = \mathbf{A} + \nabla\chi, \tag{4}$$

the gauge-invariance of the Schrödinger equation requires that the phase of the wavefunction needs to be *locally* rotated as well

$$\psi'(\mathbf{r}) = e^{i\frac{2e}{\hbar}\chi(\mathbf{r})}\psi(\mathbf{r}). \tag{5}$$

Find χ for this problem and show that the results in a) and b) are indeed connected by this gauge transformation.

Problem 2 - Second quantization and anharmonicity of the transmon (15 pts / collaboration is encouraged)

A Josephson junction shunted by a capacitor forms the simplest superconducting qubit that is named as the Cooper pair box or the transmon, depending on the parameter regime. The Hamiltonian of the circuit reads as

$$H = 4E_C(n - n_g)^2 - E_J \cos\varphi, \tag{6}$$

where n and φ are the Cooper pair number operator and the phase operator, E_C is the charging energy, E_J is the Josephson energy, and n_g is the offset charge, which will be 0 in this problem, $n_g = 0$. When the phase oscillation is small ($\langle\varphi^2\rangle \ll 2\pi$), we can approximate the system with an anharmonic oscillator by Taylor-expanding the $\cos\phi$ operator

$$H \approx 4E_C n^2 + \frac{1}{2}E_J\varphi^2 - \frac{1}{24}E_J\varphi^4. \tag{7}$$

a) Here, we assume that the dominant term is the harmonic potential ($H_0 = 4E_C n^2 + \frac{1}{2}E_J\varphi^2$), while the fourth order term is a perturbation ($V = -\frac{1}{24}E_J\varphi^4$). We can introduce creation ($a^\dagger$) and annihilation (a) operators to transform the Hamiltonian into a second quantized form:

$$\begin{aligned} n &= n_{\mathrm{ZPF}} \times i(a^\dagger - a), \\ \varphi &= \varphi_{\mathrm{ZPF}} \times (a^\dagger + a), \end{aligned} \tag{8}$$

where the zero-point fluctuations are $n_{\mathrm{ZPF}} = [E_J/(32E_C)]^{1/4}$ and $\varphi_{\mathrm{ZPF}} = [2E_C/E_J]^{1/4}$. Show that the creation and annihilation satisfy the usual commutation relation, i.e. $[a, a^\dagger] = 1$, and the harmonic part of the Hamiltonian is

$$H_0 = \hbar\omega(a^\dagger a + \frac{1}{2}), \tag{9}$$

where the transition frequency is $\omega = \sqrt{8E_C E_J}/\hbar$.

b) The effect of the higher order terms can be taken into account by using first-order perturbation theory. If $|m\rangle$ is the mth eigenstate of the Hamiltonian, the perturbation changes its energy with $\delta E_m = \langle m|V|m\rangle$. Find this correction for the first three energy levels, and determine the anharmonicity of the Cooper pair box, $\alpha = E_{21} - E_{10}$ (where the second transition is $E_{21} = E_2 - E_1$, and the first transition is $E_{10} = E_1 - E_0$). *Hint:* $a^\dagger|m\rangle = \sqrt{m+1}|m+1\rangle$ and $a|m\rangle = \sqrt{m}|m-1\rangle$.

Problem 3 - The transmon in charge basis (20 pts / collaboration is encouraged)

The Hamiltonian of the Cooper pair box in the charge basis is

$$H = 4E_C\sum_n (n - n_g)^2|n\rangle\langle n| - \frac{E_J}{2}\sum_n \left[|n+1\rangle\langle n| + |n-1\rangle\langle n|\right], \tag{10}$$

where E_C is the charging energy, E_J is the Josephson energy, and n_g is the offset charge.

a) Solve numerically the Hamiltonian and plot the energy dispersion as a function of offset charge ($n_g = -0.5 \ldots 0.5$) for the lowest lying five states. Assume the following values for the circuits $E_C/h = 0.2$ GHz and $E_J/h = 5$ GHz. *Hint:* You need to write down the Hamiltonian in a matrix form, after truncating the number operator between, for example, $n = -10$ and 10. In this case your matrices will have size of 21x21. The matrix form of the first term is diagonal, while the second term is off-diagonal. Then, you need to find the eigenvalues of the matrix as a function of the offset charge.

b) Plot the qubit eigenfunctions in this charge basis at $n_g = 0$.

Alternative Homework
(40 pts / no collaboration, instead of solving Problems 1-2-3)

1. Explain the basics of superconductivity, discuss the main properties of a superconductor, and the idea of the macroscopic wavefunction (2 pages, single spaced).
2. Derive the circuit quantization of the transmon in the presence of gate voltages. Sketch the energy levels, and the qubit wavefunctions both in charge and flux bases (2 pages, single spaced).