Paris-Saclay

Macroscopic Quantum Phenomena

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1 Quantum Information

Any two-level system can be a qubit, but real qubits always interact with the environment. In this part, we shall see how to characterize qubits and their behaviors in an open system.

1.1 Classical and Quantum Magnetic Moments: Single Qubits

1.1.1 Ammonia Molecule

The ammonia molecule (NH_3) can be viewed as a simple two-level system where two states corresponds to nitrogen atoms above or below the hydrogen plane, then the Hamiltonian can be taken as

$$H = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}, \tag{1.1}$$

its eigenvalues are

$$\lambda_\pm = E_0 \pm A, \tag{1.2}$$

and the eigenvectors are

$$|\chi_+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad |\chi_-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{1.3}$$

We find the sign of the off-diagonal elements are related to the parities of the two states. In particular, with negative off-diagonal elements we find the ground state is formed by the even-parity state, align with our intuition.

1.1.2 Classical Moment in a Magnetic Moment

Denote $\boldsymbol{\mu}$ a magnetic moment and $\boldsymbol{L}$ the angular momentum, then classically we have

$$\boldsymbol{\mu} = \gamma \boldsymbol{L}. \tag{1.4}$$

Assume no dissipation, when placed in a magnetic field $\boldsymbol{B}$, there should be

$$\frac{\mathrm{d}\boldsymbol{L}}{\mathrm{d}t} = \boldsymbol{\mu} \times \boldsymbol{B} \Leftrightarrow \frac{\mathrm{d}\boldsymbol{\mu}}{\mathrm{d}t} = \gamma \boldsymbol{\mu} \times \boldsymbol{B}. \tag{1.5}$$

Align $\boldsymbol{B}$ to the z-axis without a loss in generality, then

$$\boldsymbol{B} \cdot \frac{\mathrm{d}\boldsymbol{\mu}}{\mathrm{d}t} = \gamma \boldsymbol{B} \cdot (\boldsymbol{\mu} \times \boldsymbol{B}) = 0, \tag{1.6}$$

hence the motion of the moment is only on the xy-plane. Besides, it's obvious to verify the moment's modulus is also conserved.

We can just solve this equation of motion by writing

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix} = \gamma\begin{pmatrix}0 & B\\ -B & 0\end{pmatrix}\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix}. \tag{1.7}$$

Solve it, we immediately have

$$\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix} = \begin{pmatrix}\cos(\gamma Bt) & \sin(\gamma Bt)\\ -\sin(\gamma Bt) & \cos(\gamma Bt)\end{pmatrix}\begin{pmatrix}\mu_x(0)\\ \mu_y(0)\end{pmatrix}. \tag{1.8}$$

Now let's introduce some dynamics: Make the magnetic field rotating! Take

$$\boldsymbol{B} = B_0\hat{z} + B_1\cos(\omega t)\hat{x} + B_1\sin(\omega t)\hat{y}. \tag{1.9}$$

The trick for solving it is changing to the rotating frame, where we have

$$\frac{\mathrm{d}\boldsymbol{\mu'}}{\mathrm{d}t} = \frac{\mathrm{d}\boldsymbol{\mu}}{\mathrm{d}t} + \omega\hat{z}\times\boldsymbol{\mu} = \gamma\boldsymbol{\mu}\times(\boldsymbol{B}_0 + \boldsymbol{B_1}) + \omega\hat{z}\times\boldsymbol{\mu}. \tag{1.10}$$

After some algebra, we find

$$\frac{\mathrm{d}\boldsymbol{\mu'}}{\mathrm{d}t} = (\omega_L - \omega)\boldsymbol{\mu'}\times\hat{z} + \omega_1\boldsymbol{\mu'}\times\hat{x}', \tag{1.11}$$

where $\omega_L \equiv \gamma B_0$, $\omega_1 \equiv \gamma B_1$. In the rotating frame, we find the magnetic moment moves in an effective magnetic field

$$\gamma\boldsymbol{B}_{\text{eff}} \equiv (\omega_L - \omega)\hat{z} + \omega_1\hat{x}. \tag{1.12}$$

Assuming $\omega_1 \ll (\omega_L - \omega)$, then the previous case is recovered. While if $\omega \approx \omega_L$, we find the x-component dominants, and the magnetic field induced a magnetic moment flip w.r.t. the z-axis can be interpreted as a qubit transition $|0\rangle \to |1\rangle$.

If the magnetic moment interacts with the environment, we can phenomenologically introduce the relaxation time T_1 and the coherence time T_2, then the EoM for a $\boldsymbol{\mu}$ moving in the static magnetic field $\boldsymbol{B} = B_0\hat{z}$ acquires an additional terms related to dissipation.

T_1 characterizes $\boldsymbol{\mu}$ relaxing to its equilibrium configuration $\boldsymbol{\mu}_0$ pointing along z, we just write the term associated to it as

$$\frac{\mathrm{d}\mu_z}{\mathrm{d}t} = \frac{\mu_0 - \mu_z}{T_1}, \tag{1.13}$$

the solution writes

$$\mu_z(t) = \mu_z(0) - [\mu_z(0) - \mu_z](1 - e^{-t/T_1}). \tag{1.14}$$

T_2 characterizes the relaxation for x and y components, we assume

$$\frac{\mathrm{d}\boldsymbol{\mu}_\parallel}{\mathrm{d}t} = \gamma\boldsymbol{\mu}_\parallel \times \boldsymbol{B} - \frac{1}{T_2}\boldsymbol{\mu}_\parallel. \tag{1.15}$$

Let's assume $\mu_z \approx \mu_0$ while $\mu_x, \mu_y \ll \mu_0$, hence the μ_z dynamics decouples from $\boldsymbol{\mu}_\parallel$ dynamics, and the $\boldsymbol{\mu}_\parallel$ EoM neatly writes

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix} = \begin{pmatrix}-1/T_2 & \gamma B_0\\ -\gamma B_0 & -1/T_2\end{pmatrix}\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix}, \tag{1.16}$$

we can readily solve it:

$$\begin{pmatrix}\mu_x(t)\\ \mu_y(t)\end{pmatrix} = e^{-t/T_2}\begin{pmatrix}\cos(\gamma B_0 t) & \sin(\gamma B_0 t)\\ -\sin(\gamma B_0 t) & \cos(\gamma B_0 t)\end{pmatrix}\begin{pmatrix}\mu_x(0)\\ \mu_y(0)\end{pmatrix}. \tag{1.17}$$

1.1.3 Exercise: Classical Moment in a Rotating Magnetic Field

Here, we provide the solution for Exercise 1.1.

1. Since

$$\frac{\mathrm{d}\boldsymbol{\mu}_\parallel}{\mathrm{d}t} = \gamma(\boldsymbol{\mu} \times \boldsymbol{B})_\parallel - \frac{\boldsymbol{\mu}_\parallel}{T_1}, \tag{1.18}$$

and under the assumption that $\mu_z = \mu_0 = Const$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix} = \begin{pmatrix}-1/T_1 & \gamma B_0\\ -\gamma B_0 & -1/T_1\end{pmatrix}\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix} + \gamma\mu_0 B_1\begin{pmatrix}\sin(\omega t)\\ \cos(\omega t)\end{pmatrix}. \tag{1.19}$$

Denote $\omega_L \equiv \gamma B_0$ and notice that with the unitary matrix

$$U \equiv \frac{1}{\sqrt{2}}\begin{pmatrix}-\mathrm{i} & 1\\ \mathrm{i} & 1\end{pmatrix}, \tag{1.20}$$

we can diagonalize the matrix to

$$U\begin{pmatrix}-1/T_1 & \gamma B_0\\ -\gamma B_0 & -1/T_1\end{pmatrix}U^\dagger = \begin{pmatrix}-\Gamma - \mathrm{i}\omega_L & 0\\ 0 & -\Gamma + \mathrm{i}\omega_L\end{pmatrix}, \tag{1.21}$$

where $\Gamma \equiv 1/T_2$. Denote

$$U\begin{pmatrix}\mu_x\\ \mu_y\end{pmatrix} = \begin{pmatrix}(-\mathrm{i}\mu_x + \mu_y)/\sqrt{2}\\ (\mathrm{i}\mu_x + \mu_y)/\sqrt{2}\end{pmatrix} \equiv \begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} \tag{1.22}$$

We then have

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix}-\Gamma - \mathrm{i}\omega_L & 0\\ 0 & -\Gamma + \mathrm{i}\omega_L\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} + \frac{\gamma\mu_0 B_1}{\sqrt{2}}\begin{pmatrix}e^{-\mathrm{i}\omega t}\\ e^{\mathrm{i}\omega t}\end{pmatrix}. \tag{1.23}$$

We find the equation of motion for α and β are conjugate, we only need to consider the one for α:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = (-\Gamma - \mathrm{i}\omega_L)\alpha + \frac{\gamma\mu_0 B_1}{\sqrt{2}} e^{-\mathrm{i}\omega t}. \tag{1.24}$$

The inhomogeneous term can be eliminated by the ansatz

$$\alpha(t) = A(t) + ke^{-\mathrm{i}\omega t}. \tag{1.25}$$

Inserting it back to the EoM, we find

$$\frac{\mathrm{d}A}{\mathrm{d}t} = (-\Gamma - \mathrm{i}\omega_L)A + \left(\frac{\gamma\mu_0 B_1}{\sqrt{2}} - [\Gamma + \mathrm{i}(\omega_L - \omega)]k\right)e^{-\mathrm{i}\omega t}. \tag{1.26}$$

We only need to set

$$k = \frac{\gamma\mu_0 B_1}{\sqrt{2}[\Gamma + \mathrm{i}(\omega_L - \omega)]}, \tag{1.27}$$

and the solution writes

$$\alpha(t) = A_0 e^{-\Gamma t} e^{-\mathrm{i}\omega_L t} + \frac{\gamma\mu_0 B_1}{\sqrt{2}[\Gamma + \mathrm{i}(\omega_L - \omega)]} e^{-\mathrm{i}\omega t}, \tag{1.28}$$

$$\beta(t) = \alpha^*(t) = A_0^* e^{-\Gamma t} e^{\mathrm{i}\omega_L t} + \frac{\gamma\mu_0 B_1}{\sqrt{2}[\Gamma - \mathrm{i}(\omega_L - \omega)]} e^{\mathrm{i}\omega t}. \tag{1.29}$$

Since

$$\mu_x = \frac{\mathrm{i}}{\sqrt{2}}(\alpha - \beta) = -\sqrt{2}\,\mathrm{Im}\,\alpha, \quad \mu_y = \frac{1}{\sqrt{2}}(\alpha + \beta) = \sqrt{2}\,\mathrm{Re}\,\alpha, \tag{1.30}$$

and notice

$$\begin{aligned}
&\frac{\gamma\mu_0 B_1}{\sqrt{2}[\Gamma + \mathrm{i}(\omega_L - \omega)]} e^{-\mathrm{i}\omega t} = \frac{\gamma\mu_0 B_1}{\sqrt{2}} \frac{[\Gamma - \mathrm{i}(\omega_L - \omega)]}{\Gamma^2 + (\omega_L - \omega)^2} [\cos(\omega t) - \mathrm{i}\sin(\omega t)] \\
&= \frac{\gamma\mu_0 B_1}{\sqrt{2}[\Gamma^2 + (\omega_L - \omega)^2]} \{[\Gamma\cos(\omega t) - (\omega_L - \omega)\sin(\omega t)] - \mathrm{i}[\Gamma\sin(\omega t) + (\omega_L - \omega)\cos(\omega t)]\},
\end{aligned} \tag{1.31}$$

then

$$\mu_x = -\sqrt{2}e^{-\Gamma t}\,\mathrm{Im}(A_0 e^{-\mathrm{i}\omega_L t}) + \frac{\gamma\mu_0 B_1}{\Gamma^2 + (\omega_L - \omega)^2}[\Gamma\sin(\omega t) + (\omega_L - \omega)\cos(\omega t)], \tag{1.32}$$

$$\mu_y = \sqrt{2}e^{-\Gamma t}\,\mathrm{Re}(A_0 e^{-\mathrm{i}\omega_L t}) + \frac{\gamma\mu_0 B_1}{\Gamma^2 + (\omega_L - \omega)^2}[\Gamma\cos(\omega t) - (\omega_L - \omega)\sin(\omega t)]. \tag{1.33}$$

2.

3. In steady regime, the first terms are exponentially suppressed and we only need to

consider the second term. The instantaneous power writes

$$P(t) = -\boldsymbol{\mu}_{\parallel} \cdot \frac{\mathrm{d}\boldsymbol{B}_1}{\mathrm{d}t} = \frac{\gamma\mu_0\omega B_1^2}{\Gamma^2 + (\omega_L - \omega)^2}\Gamma. \tag{1.34}$$

1.1.4 Quantum Spins in a Rotating Magnetic Field

Our convention on Pauli matrices is

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.35}$$

In general, the Hamiltonian for a spin in a magnetic field writes

$$H = -\boldsymbol{\mu} \cdot \boldsymbol{B}, \quad \boldsymbol{\mu} \equiv \gamma \boldsymbol{S} = \frac{\hbar\gamma}{2}\boldsymbol{\sigma}. \tag{1.36}$$

For a rotating magnetic field, we denote

$$\boldsymbol{B} = B_0\hat{z} + B_1\cos(\omega t)\hat{x} - B_1\sin(\omega t)\hat{y}, \tag{1.37}$$

now the Hamiltonian writes

$$H = -\frac{\hbar\gamma}{2}\begin{pmatrix} B_0 & B_1 e^{+\mathrm{i}\omega t} \\ B_1 e^{-\mathrm{i}\omega t} & B_0 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} \omega_L & \omega_1 e^{\mathrm{i}\omega t} \\ \omega_1 e^{-\mathrm{i}\omega t} & -\omega_L \end{pmatrix}. \tag{1.38}$$

The trick tackling this problem is again changing to the rotating frame. Now we have to consider the $\mathsf{SU}(2)$ matrix generated by α rotation around the rotation axis $\hat{n}$,

$$R(\alpha) = \exp\left(-\frac{\mathrm{i}}{2}\alpha\boldsymbol{\sigma}\cdot\hat{n}\right), \tag{1.39}$$

now α is time-dependent like ωt, hence

$$U(t) \equiv R(\omega t) = \exp\left(-\frac{\mathrm{i}}{2}\omega t\sigma_z\right) = \begin{pmatrix} e^{-\frac{\mathrm{i}}{2}\omega t} & 0 \\ 0 & e^{\frac{\mathrm{i}}{2}\omega t} \end{pmatrix}. \tag{1.40}$$

Note $U(t)$ has time dependence, hence the Schrödinger equation

$$H\left|\psi\right\rangle = \mathrm{i}\hbar\partial_t\left|\psi\right\rangle \tag{1.41}$$

makes the unitary transformation on H be

$$H \to H' = UHU^\dagger - \mathrm{i}\hbar U\partial_t U^\dagger, \tag{1.42}$$

and

$$(UHU^\dagger - \mathrm{i}\hbar U\partial_t U^\dagger)(U\left|\Psi\right\rangle) = \partial_t(U\left|\Psi\right\rangle). \tag{1.43}$$

Explicit calculation shows

$$H' = \frac{\hbar}{2}\begin{pmatrix} \omega - \omega_L & -\omega_1 \\ -\omega_1 & -(\omega - \omega_L) \end{pmatrix} \equiv \frac{\hbar}{2}\begin{pmatrix} \delta & -\omega_1 \\ -\omega_1 & -\delta \end{pmatrix}, \tag{1.44}$$

where we denote $\delta = \omega - \omega_L$. Immediately, we find its eigenalues are

$$\mathcal{E}_\pm = \pm\frac{\hbar}{2}\sqrt{\delta^2 + \omega_1^2} \equiv \pm\frac{\hbar}{2}\Omega, \tag{1.45}$$

where $\Omega \equiv \sqrt{\delta^2 + \omega_1^2}$. The corresponding eigenvectors are

$$|\psi_+\rangle \propto \begin{pmatrix} \dfrac{-\delta - \Omega}{\omega_1} \\ 1 \end{pmatrix}, \quad |\psi_-\rangle \propto \begin{pmatrix} \dfrac{-\delta + \Omega}{\omega_1} \\ 1 \end{pmatrix}. \tag{1.46}$$

We shall formally denote the nomralized eigenvectors as

$$|\psi_+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}, \quad |\psi_-\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}. \tag{1.47}$$

Actually, we can always ensure such a form for eigenvectors for real-eigensystem Hamiltonians. For our case here,

$$\theta \equiv 2\arctan\frac{-\omega}{\delta + \Omega}. \tag{1.48}$$

Suppose we prepare the system in a state $|\psi_0'(t=0)\rangle$ and its the same as the state in the rotating frame, we denote

$$|\psi(0)\rangle = \big|\psi'(0)\big\rangle = |0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{1.49}$$

The question is, at a later time t, what's the probability of finding the state in the state

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1.50}$$

The time-evolution of the initial state $|\psi(0)\rangle$ in the rotating frame is immediately given by

$$|\psi(t)\rangle = e^{-\mathrm{i}\frac{\Omega}{2}t}\cos\frac{\theta}{2}\,|\psi_+\rangle - e^{+\mathrm{i}\frac{\Omega}{2}t}\sin\frac{\theta}{2}\,|\psi_-\rangle\,. \tag{1.51}$$

The amplitude reaching $|1\rangle$ state at t then writes

$$\mathcal{A}(t) = (e^{-\mathrm{i}\frac{\Omega}{2}t} - e^{+\mathrm{i}\frac{\Omega}{2}t})\sin\frac{\theta}{2}\cos\frac{\theta}{2} = -\mathrm{i}\sin\left(\frac{\Omega}{2}t\right)\sin\theta, \tag{1.52}$$

and the probability writes

$$P_{0\to1}(t) = \sin^2\left(\frac{\Omega}{2}t\right)\sin^2\theta = \frac{\tan^2\theta}{1+\tan^2\theta}\sin^2\frac{\Omega t}{2}. \tag{1.53}$$

This is exactly the Rabi oscillation. Note the probability is the same whether in the lab frame or the rotating frame, since states in the two frames are related by a global unitary transformation and these two frames are simultaneous.

Note

$$\tan\frac{\theta}{2} = -\frac{\omega_1}{\delta+\Omega}, \tag{1.54}$$

hence

$$\tan\theta = \frac{2\tan\frac{\theta}{2}}{1-\tan^2\frac{\theta}{2}} = -\frac{2\omega_1(\delta+\Omega)}{(\delta+\Omega)^2-\omega_1} = -\frac{\omega_1}{\delta}, \tag{1.55}$$

and

$$P_{0\to1}(t) = \frac{\omega_1^2}{\omega_1^2+\delta^2}\sin^2\frac{\Omega t}{2}. \tag{1.56}$$

At resonance, $\delta = \omega - \omega_L = 0$, and we find

$$P_{0\to1} = \sin^2\frac{\omega_1 t}{2}, \tag{1.57}$$

and it could reach 1 at certain time. If we are off-resonance, clearly $P_{0\to1}$ can never reach 1.

We can impose a similar phenomenological approach as the Bloch's treatment for classical spins to quantum spins. We assume $|0\rangle$ and $|1\rangle$ are metastable with a lifetime τ. In this case, for an ensemble of quantum objects, there exist a leakage to the environment hence the system is open. Suppose we have prepared the ensemble to be populated in state $|0\rangle$, now we wish to study its transitions to $|1\rangle$.

Intuitively, the expected number of transitions is

$$N_{01}(t) = n\int_0^\infty \mathrm{d}t\; P_{0\to1}(t)e^{-t/\tau} = \frac{n}{2\Gamma}\frac{\omega_1^2}{\delta^2+\omega_1^2+\Gamma^2}, \quad \Gamma \equiv \frac{1}{\tau}. \tag{1.58}$$

It has a Lorenzian lineshape, and the FWHM writes

$$\mathrm{FWHM} = \sqrt{\omega_1^2+\Gamma^2}. \tag{1.59}$$

Experimentally, we can measure the FWHM for different values of ω_1 and extrapolate to obtain Γ.

1.1.5 Density Matrices

A pure state of a quantum system can be written as a linear combination of eigenstates. For a qubit, a general pure state can always be written as

$$|\psi\rangle = a|0\rangle + b|1\rangle, \qquad a, b, \in \mathbb{C}. \tag{1.60}$$

A mixed state, however, is a statisitcal mixture of different pure states, we can define it as a set of tuples $\mathcal{M} = \{(|\psi_i\rangle, p_i)\}$, where p_i is the probability finding the system in the state $|\psi_i\rangle$ and clearly we demand a normalized probability

$$\sum_i p_i = 1. \tag{1.61}$$

Obviously, a pure state is merely a special mixed state.

For a mixed state $\mathcal{M}$, its density matrix is defined to be

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|. \tag{1.62}$$

Given a density matrix ρ, the probability of being in some state $|\psi_n\rangle$ neatly writes $\langle\psi_n|\rho|\psi_n\rangle$, and we clearly have

$$\operatorname{tr}\rho = 1. \tag{1.63}$$

Besides, the definition implies ρ is semi-definite positive, in the sense that it only have non-zero eigenvalues. Conversely, we can identify any semi-positive definite operator with normalized trace as a density matrix. Apparently, according to the definition, we also have

$$\det\rho = 0 \tag{1.64}$$

only for pure states. Besides,ρ can be viewed as a projective operator

$$\rho^2 = \rho. \tag{1.65}$$

The expectation value for an observable A then can be written as

$$\langle A\rangle = \operatorname{tr}(A\rho). \tag{1.66}$$

According to Schrödinger equation, the von Neumann equation determining the time-evolution for a dentisy matrix $\rho(t)$ can be easily derived:

$$\mathrm{i}\hbar\partial_t\rho = [H, \rho]. \tag{1.67}$$

Since density matrices describes the system equally well as common wavefunctions, in quantum information jargon, we will also refer to ρ as a "state".

1.1.6 Spins in a Noisy Magnetic Field

Now let's consider a spin in a noisy magnetic field pointed along z-direction, and the Hamiltonian writes

$$H = -\boldsymbol{\mu}\cdot\boldsymbol{B} = -\frac{\hbar}{2}\begin{pmatrix}\omega_L(t) & 0\\ 0 & -\omega_L(t)\end{pmatrix}, \tag{1.68}$$

where $\omega_L(t)$ has a random time-dependence. Denote tha state of our system as

$$|\psi(t)\rangle = \begin{pmatrix} \lambda(t) \\ \kappa(t) \end{pmatrix}, \tag{1.69}$$

the Schrödinger equation then writes

$$\mathrm{i}\hbar\partial_t\lambda(t) = -\frac{\hbar}{2}\omega_L(t)\lambda(t), \qquad \mathrm{i}\hbar\partial_t\kappa(t) = \frac{\hbar}{2}\omega_L(t)\kappa(t). \tag{1.70}$$

The formal solution writes

$$\lambda(t) = \exp\left(\frac{\mathrm{i}}{2}\int_0^t \mathrm{d}t\ \omega_L(t)\right)\lambda_0, \qquad \kappa(t) = \exp\left(-\frac{\mathrm{i}}{2}\int_0^t \mathrm{d}t\ \omega_L(t)\right)\kappa_0. \tag{1.71}$$

The density matrix for $|\psi\rangle$ then writes

$$\rho = \begin{pmatrix} |\lambda_0|^2 & e^{\mathrm{i}\int_0^t \mathrm{d}t\ \omega_L(t)}\lambda_0\kappa_0^* \\ e^{-\mathrm{i}\int_0^t \mathrm{d}t\ \omega_L(t)}\lambda_0^*\kappa_0 & |\kappa_0|^2. \end{pmatrix} \tag{1.72}$$

We now find the existence of non-trivial off-diagonal terms, which are conventionally callede coherences.

We assume $\omega_L(t)$ is sampled from a stationary Gaussian distribution $\mathcal{N}(\omega_L^0, \sigma_\omega)$. Assuming ω_L at different times are weakly correlated, then we have

$$C(t,t') \equiv \overline{\omega_L(t)\omega_L(t')} - \overline{\omega_L(t)}\ \overline{\omega(t')} \equiv g(|t-t'|), \tag{1.73}$$

where $g(|t-t'|)$ peaks at $t=t'$ but decays to 0 for $|t-t'| \gg 1$, we shall adpot

$$g(|t-t'|) = Ge^{-|t-t'|/\tau}. \tag{1.74}$$

Now we can separate $\omega_L(t)$ to be

$$\omega_L(t) = \omega_L^0 + \delta\omega_L(t), \tag{1.75}$$

and we immediately find

$$\overline{\delta\omega_L(t)\delta\omega_L(t')} = g(|t-t'|). \tag{1.76}$$

Now let's treat the stochastic phase factor in the density matrix: Take the lower-left element as example, factorizing the fluctuating part, we find

$$e^{-\mathrm{i}\int_0^t \mathrm{d}t\ \omega_L(t)} = e^{-\mathrm{i}\omega_L^0 t}e^{-\mathrm{i}\int_0^t \mathrm{d}t\ \delta\omega_L(t)}. \tag{1.77}$$

Let's consider the enemble average, and notice

$$\overline{\exp(A)} = \sum_{n=0}^{\infty}\frac{1}{n!}\overline{A^n}. \tag{1.78}$$

Assuming $A \in \mathcal{N}(0,\sigma)$ and by Wick theorem we have

$$\overline{\exp(A)} = \sum_{n=0}^{\infty} \frac{1}{(2n)!}\overline{A^{2n}} = \sum_{n=0}^{\infty} \frac{(2n-1)!!}{(2n)!}(\overline{A^2})^n = \sum_{n=0}^{\infty} \frac{1}{n!2^n}(\overline{A^2})^n = \exp\left(\frac{1}{2}\overline{A^2}\right). \tag{1.79}$$

Now we find

$$\overline{e^{-\mathrm{i}\int_0^t \mathrm{d}t\, \omega_L(t)}} = e^{-\mathrm{i}\omega_L^0 t} e^{-\frac{1}{2}\int_0^t \mathrm{d}t'\mathrm{d}t'' g(|t'-t''|)}. \tag{1.80}$$

Inserting the ansatz for $g(|t-t'|)$ and completing the integration, we find

$$\int_0^t \mathrm{d}t'\mathrm{d}t'' g(|t'-t''|) = 2G[\tau t - \tau^2(1-e^{-t/\tau})], \tag{1.81}$$

hence

$$\overline{e^{-\mathrm{i}\int_0^t \mathrm{d}t\, \omega_L(t)}} = e^{-\mathrm{i}\omega_L^0 t} e^{G(\tau^2 - t\tau - \tau^2 e^{-t/\tau})}. \tag{1.82}$$

For $t \gg \tau$, we have

$$\overline{e^{-\mathrm{i}\int_0^t \mathrm{d}t\, \omega_L(t)}} \approx e^{-\mathrm{i}\omega_L^0 t} e^{-G\tau(t-\tau)}. \tag{1.83}$$

This implies the off-diagonal term is exponentially suppressed, hence the noise induces a quantum decoherence/phase damping. Such decoherence reduces entanglements in our system, and makes our system more "classical".

1.1.7 Exercise 1.2

The total Hamiltonian writes

$$H = \begin{pmatrix} E - \frac{\mathrm{i}\hbar}{2}\Gamma & A \\ A & E \end{pmatrix}, \tag{1.84}$$

and the secular equation writes

$$\left(\lambda - E + \frac{\mathrm{i}\hbar}{2}\Gamma\right)(\lambda - E) - A^2 = 0, \tag{1.85}$$

$$\lambda^2 - \left(2E - \frac{\mathrm{i}\hbar}{2}\Gamma\right)\lambda + E\left(E - \frac{\mathrm{i}\hbar}{2}\Gamma\right) - A^2 = 0, \tag{1.86}$$

$$\begin{aligned} \lambda_\pm &= E - \frac{\mathrm{i}\hbar}{4}\Gamma \pm \frac{1}{2}\sqrt{\left(2E - \frac{\mathrm{i}\hbar}{2}\Gamma\right)^2 - 4E\left(E - \frac{\mathrm{i}\hbar}{2}\Gamma\right) + 4A^2} \\ &= E - \frac{\mathrm{i}\hbar}{4}\Gamma \pm \sqrt{A^2 - \frac{\hbar^2}{16}\Gamma^2}. \end{aligned} \tag{1.87}$$

For $|\psi_+\rangle$, consider

$$\begin{pmatrix} -\frac{\mathrm{i}\hbar}{4}\Gamma - \sqrt{A^2 - \frac{\hbar^2}{16}\Gamma^2} & A \\ A & \frac{\mathrm{i}\hbar}{4}\Gamma - \sqrt{A^2 - \frac{\hbar^2}{16}\Gamma^2} \end{pmatrix} |\psi_+\rangle = 0. \tag{1.88}$$

It's equivalent to

$$\begin{pmatrix} A\left(-\sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2}-\frac{\mathrm{i}\hbar}{4}\Gamma\right) & A^2 \\ A\left(-\sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2}-\frac{\mathrm{i}\hbar}{4}\Gamma\right) & A^2 \end{pmatrix} |\psi_+\rangle = 0, \tag{1.89}$$

and we immediately find

$$|\psi_+\rangle \propto \begin{pmatrix} A \\ \sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2}+\frac{\mathrm{i}\hbar}{4}\Gamma \end{pmatrix}. \tag{1.90}$$

Likewise, for $|\psi_-\rangle$, there should be

$$\begin{pmatrix} -\frac{\mathrm{i}\hbar}{4}\Gamma+\sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2} & A \\ A & \frac{\mathrm{i}\hbar}{4}\Gamma+\sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2} \end{pmatrix} |\psi_-\rangle = 0, \tag{1.91}$$

which equivalents to

$$\begin{pmatrix} A\left(\sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2}-\frac{\mathrm{i}\hbar}{4}\Gamma\right) & A^2 \\ A\left(\sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2}-\frac{\mathrm{i}\hbar}{4}\Gamma\right) & A^2 \end{pmatrix} |\psi_+\rangle = 0, \tag{1.92}$$

hence

$$|\psi_-\rangle \propto \begin{pmatrix} -A \\ \sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2}-\frac{\mathrm{i}\hbar}{4}\Gamma \end{pmatrix}. \tag{1.93}$$

Clearly, $|\psi_\pm\rangle$ have the same normalization factor:

$$\mathscr{N} = A\sqrt{2}, \tag{1.94}$$

hence

$$|\psi_\pm\rangle = \frac{1}{A\sqrt{2}} \begin{pmatrix} \pm A \\ \sqrt{A^2-\frac{\hbar^2}{16}\Gamma^2}\pm\frac{\mathrm{i}\hbar}{4}\Gamma \end{pmatrix}. \tag{1.95}$$

1.2 Entanglement

1.2.1 Entangled States and Product States

Consider a bipartite system and pure states, let A and B be two qubits whose Hilbert spaces are denoted as $\mathscr{H}_A$ and $\mathscr{H}_B$. Let

$$|\psi_A\rangle = \begin{pmatrix} \lambda_A \\ \mu_A \end{pmatrix}, \qquad |\psi_B\rangle = \begin{pmatrix} \lambda_B \\ \mu_B, \end{pmatrix} \tag{1.96}$$

then their tensor product $|\psi_A\rangle \otimes |\psi_B\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B$ writes

$$|\psi_A\rangle \otimes |\psi_B\rangle = \begin{pmatrix} \lambda_A\lambda_B \\ \lambda_A\mu_B \\ \mu_A\lambda_B \\ \mu_A\mu_B \end{pmatrix}. \tag{1.97}$$

Such a state in $\mathscr{H}_A \otimes \mathscr{H}_B$ can be written in terms of a single tensor product, hence is called a product state and is also called separable.

However, a general pure state $|\Psi\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B$ cannot be written as a single tensor product by one state in $\mathscr{H}_A$ and anothe in $\mathscr{H}_B$. When it is the case, we say $|\Psi\rangle$ is an entangled state. Obviously, the terminologies we introduce here can be easily generalized to an n-partite system whose Hilbert space is $\mathscr{H}^{\otimes n}$.

For example, the Bell states aree

$$|\Phi_\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle), \quad |\Psi_\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle). \tag{1.98}$$

Actually, $|\Phi_+\rangle$ characterizes the A-phase of superfluid ^{3}He, while $|\Psi_-\rangle$ gives the spin texture of Cooper pairs in a conventional superconductor.

In quantum computing jargon, a Greenburger-Horne-Zeilinger state is

$$|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle). \tag{1.99}$$

Besides, a Weiner state reads

$$|\mathrm{W}\rangle = \alpha\,|001\rangle + \beta\,|010\rangle + \gamma\,|100\rangle\,, \tag{1.100}$$

where the state normalization is assumed.

1.2.2 Schmidt Decomposition

The Schmidt decomposition serves as a test/definition for entanglement for bipartite pure states.

Theorem 1.1 (Schmidt Decomposition Theorem) *Let $\mathscr{H}_A$ be a Hilbert state of dimension m and let $\mathscr{H}_B$ be a Hilbert space of dimension n. For any pure state $|\psi\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B$, there exist an otrhonormal basis $\{|k\rangle_A\}$ for $\mathscr{H}_A$ and $\{|k\rangle_B\}$ for $\mathscr{H}_B$ s.t.*

$$|\psi\rangle = \sum_k \sigma_k\,|k\rangle_A \otimes |k\rangle_B\,, \tag{1.101}$$

where $\sigma_k \in \mathbb{R}^+$.

To prove this theorem, consider any orthonormal basis $\{|i\rangle_A\}$ for $\mathscr{H}_A$ and $\{|j\rangle_B\}$ for $\mathscr{H}_B$, we can always decompose

$$|\psi\rangle = \sum_{i,j} M_{ij}\,|i\rangle_A \otimes |j\rangle_B\,. \tag{1.102}$$

Now we find the coefficients can be organized in terms of a $m \times n$ matrix $\mathbf{M}$, and according to the singular value decomposition theorem, there exist unitary $m \times m$ and $n \times n$ matrices $\mathbf{U}, \mathbf{V}$ and a diagonal matrix $\mathbf{\Sigma}$ s.t.

$$\mathbf{M} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\dagger. \tag{1.103}$$

The diagonal $m \times n$ matrix $\mathbf{\Sigma}$ satisfies

$$\Sigma_{ii} = \sigma_i \in \mathbb{R}^+, \quad \text{for } 1 \leq i \leq \min(m, n). \tag{1.104}$$

Now let's insert the singular-value-decomposed coefficient matrix back in the ket's expression, we find

$$|\psi\rangle = \sum_k \sigma_k \sum_{i,j} U_{i,k} V^\dagger_{k,j} |i\rangle_A \otimes |j\rangle_B . \tag{1.105}$$

Once we define

$$|k_A\rangle \equiv \sum_i U_{i,k} |i\rangle_A , \qquad |k\rangle_B \equiv \sum_j V^\dagger_{k,j} |j\rangle_B , \tag{1.106}$$

the proof is completed.

Conventionally, the number of singular values of $\mathbf{M}$ is called the rank of $\mathbf{M}$, also known as the Schmidt rank or Schmidt number of $|\psi\rangle$. Clearly, a rank-1 state is separable, while higher-rank states are not.

Let's return to the simplest qubit case where a tensor product state of a bipartite system can be written as

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} . \tag{1.107}$$

Now the coefficient matrix reads

$$\mathbf{M} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} . \tag{1.108}$$

Note the Schmidt decomposition generally reads

$$\mathbf{M} = \mathbf{U} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \mathbf{V}^\dagger. \tag{1.109}$$

If the state is a product state, then one of the $\{\sigma_1, \sigma_2\}$ is zero, hence

$$\det \mathbf{M} = 0. \tag{1.110}$$

We then find a simple criterion for a qubit tensor product state be separable:

$$\alpha\delta = \beta\gamma. \tag{1.111}$$

1.2.3 Reduced Density Matrix

Consider a composite system AB described by $\mathscr{H}_A \otimes \mathscr{H}_B$, its states can always be written as

$$|\psi\rangle = \sum_{ij} c_{ij} |i\rangle_A \otimes |j\rangle_B . \tag{1.112}$$

Then the pure state density matrix writes

$$\rho_{AB} = |\psi\rangle\langle\psi| = \sum_{i,j;k,\ell} c_{ij} c^*_{k\ell} |i\rangle\langle k|_A \otimes |j\rangle\langle\ell|_B . \tag{1.113}$$

The reduced density matrix ρ_A on $\mathscr{H}_A$ is defined to be the partial trace of ρ_{AB} on $\mathscr{H}_B$, hence

$$\rho_A = \mathrm{tr}_B \, \rho_{AB} = \sum_{i,j,k} c_{ij} c^*_{kj} |i\rangle\langle k|_A . \tag{1.114}$$

The reduced density matrix on $\mathscr{H}_B$ can be similarly defined.

Now consider an operator $\hat{O}$ acting only on A, denote $\tilde{O} \equiv \hat{O} \otimes \mathbb{1}_B$. Then we find

$$\left\langle \tilde{O} \right\rangle = \mathrm{tr}\Big(\tilde{O}\rho_{AB}\Big) = \mathrm{tr}_A(\hat{O}\rho_A). \tag{1.115}$$

Hence, we find ρ_A effectively describes the subsystem A.

For example, consider $|\psi\rangle = |a\rangle \otimes |b\rangle$ as a product state, then $\rho_{AB} = |a\rangle\langle a| \otimes |b\rangle\langle b|$ and the reducde density matrix of A neatly reads $\rho_A = |a\rangle\langle a|$, which is a pure state. However, if $|\psi\rangle$ is an entagnled state (here we take it as the Bell state $|\Psi_+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$), then

$$\rho_{AB} = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11| + |00\rangle\langle 11| + |11\rangle\langle 00|), \tag{1.116}$$

hence

$$\rho_A = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|). \tag{1.117}$$

We find it describes a maximally mixed state, aligning with our intuition that the entanglement between two subsystems reduces our knowledge when only A is avaliable.

1.2.4 Qubit Representations

Let's consider linear photon representations instead of spins. Denote $|x\rangle$ and $|y\rangle$ are two linear polarization states along x or y directions. Then a general baiss linearly polarization state can be written as

$$|+,\theta\rangle = \cos\theta \, |x\rangle + \sin\theta \, |y\rangle , \tag{1.118}$$

$$|-,\theta\rangle = -\sin\theta \, |x\rangle + \cos\theta \, |y\rangle . \tag{1.119}$$

As we know, a general qubit state writes

$$|\psi\rangle = \lambda \, |0\rangle + \mu \, |1\rangle , \quad |\lambda|^2 + |\mu|^2 = 1. \tag{1.120}$$

In general, $\lambda, \mu \in \mathbb{C}$, hence we can conveniently denote them as

$$\lambda = \cos\frac{\theta}{2}e^{-\mathrm{i}\phi/2}, \qquad \mu = \sin\frac{\theta}{2}e^{\mathrm{i}\phi/2}, \tag{1.121}$$

note we can always redefine the global phase so that the augments for λ and μ are opposite. Under such a coefficient parameterization, ϕ can be viewed as a elliptically polarized light corresponding to a point on the Bloch sphere — physically it correspondss to a unit-length spin pointing to the direction (θ, ϕ) in $\mathbb{R}^3$.

A spin in a magnetic field pointing along $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the Hamiltonian writes

$$H \sim \boldsymbol{\sigma}\cdot\hat{n} = \begin{pmatrix} \cos\theta & e^{-\mathrm{i}\phi}\sin\theta \\ e^{\mathrm{i}\phi}\sin\theta & -\cos\theta \end{pmatrix}, \tag{1.122}$$

and the $|\psi\rangle$ state constructed above is an eigenstate of it.

1.2.5 Einstein-Poldolsky-Rosen Paradox

Suppose two photons A and B are prepared in the polarization state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|x\rangle_A \otimes |x\rangle_B + |y\rangle_A \otimes |y\rangle_B), \tag{1.123}$$

and they are sent along opposite directions to two observers, here denoted as Alice and Bob. These two observers measure the polarization using two polarizers aligned along θ_A and θ_B w.r.t. the x-axis, hence the eigenstates for the two polarizers write

$$\begin{pmatrix} |A/B_+\rangle \\ |A/B_-\rangle \end{pmatrix} = \begin{pmatrix} \cos\theta_{A/B} & \sin\theta_{A/B} \\ -\sin\theta_{A/B} & \cos\theta_{A/B} \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \end{pmatrix} \tag{1.124}$$

Now we are interested in the probabilities of all possible joint measure outcomes, which is eeasy to compute:

$$P(++) = P(--) = \frac{1}{2}\cos^2(\theta_A - \theta_B), \tag{1.125}$$

$$P(+-) = P(-+) = \frac{1}{2}\sin^2(\theta_A - \theta_B). \tag{1.126}$$

We find regardeless of the value of θ_A, θ_B, half of the photons will be measured along $|A/B_+\rangle$ and half along $|A/B_-\rangle$.

We can define the degree of correlation as

$$E_{AB}^{\mathrm{QM}} \equiv P(++) + P(--) - P(+-) - P(-+) = \cos[2(\theta_A - \theta_B)]. \tag{1.127}$$

When it's the case for $\theta_A = \theta_B$, then we find $E_{AB}^{\mathrm{QM}} = 1$, hence their measurements are perfectly correlated for whatever distance between Alice and Bob. In particular, this correlation seems to be instantaneous and faster than c — a paradox!

1.2.6 Hidden Variable Theory

Suppose there exists a hidden variable λ giving the polarization of the two photons separately such that there are functions

$$A(\vec{a},\lambda)=\pm 1,\qquad B(\vec{b},\lambda)=\pm 1, \tag{1.128}$$

giving the possible measure outcomes for the two observers.

λ is determined by the shource and confers to a probability distribution $\rho(\lambda)$, then the joint probability reads

$$P(\pm\pm)=\frac{1}{4}\int \mathrm{d}\lambda\ \rho(\lambda)[1\pm A(\vec{a},\lambda)][1\pm B(\vec{b},\lambda)]. \tag{1.129}$$

Then the correlation function reads

$$E_{AB}^{\mathrm{HV}}=\int \mathrm{d}\lambda\ \rho(\lambda)A(\vec{a},\lambda)B(\vec{b},\lambda). \tag{1.130}$$

Suppose two emitted photons has the same polarization and the hidden variable λ is chosen to be the polarization angle sampling from

$$\rho(\lambda)=\frac{1}{2\pi}, \tag{1.131}$$

and

$$A(\vec{a},\lambda)\equiv \mathrm{sgn}[\cos(2\theta_a-2\lambda)],\quad B(\vec{b},\lambda)\equiv \mathrm{sgn}[\cos(2\theta_b-2\lambda)]. \tag{1.132}$$

In this way, we find

$$P_A(\pm)=P_B(\pm)=\frac{1}{2}, \tag{1.133}$$

agrees with the EPR gedanken result. However, the correlation function now reads

$$E_{AB}^{\mathrm{HV}}=1-\frac{4}{\pi}|\theta_A-\theta_B|. \tag{1.134}$$

Although this doesn't match the correlation function given by quantum mechanics, but we cannot rule out the possibility that other hidden-variable theory might be able to mimic QM.

1.2.7 CHSH Theorem

Consider two polarizations for A, denoted as $\vec{a}$ and $\vec{a}'$; also two polarizations for B, $\vec{b}$ and $\vec{b}'$. Suppose the measurement is deterministic w.r.t. a hidden variable λ, then we denote the measuring outcomes as $A_\lambda\equiv A(\vec{a},\lambda)$, $A'_\lambda\equiv A(\vec{a}',\lambda)$, $B_\lambda\equiv B(\vec{b},\lambda)$, $B'_\lambda\equiv B(\vec{b},\lambda)$. Define the correlation function

$$\sigma_{AB}(\vec{a},\vec{a}';\vec{b},\vec{b}';\lambda)\equiv AB-AB'+A'B+A'B'=A(B-B')+A'(B+B')\in\{\pm 2,0\}. \tag{1.135}$$

Hence we find

$$-2 \leq \int \mathrm{d}\lambda \rho(\lambda) \sigma_{AB}(\vec{a}, \vec{a}'; \vec{b}, \vec{b}'; \lambda) \leq 2, \tag{1.136}$$

but it's nothing more than

$$S_{AB}^{\mathrm{HV}} \equiv E_{AB}^{\mathrm{HV}}(a, b) - E_{AB}^{\mathrm{HV}}(a, b') + E_{AB}^{\mathrm{HV}}(a', b) + E_{AB}^{\mathrm{HV}}(a', b') \in [-2, 2]. \tag{1.137}$$

This version of Bell's theorem is Clauser-Horne-Simony-Hott (CHSH) theorem, this should be true for all hidden variable theories.

The CHSH theorem can be violated in quantum mechanics, where

$$E_{AB}^{\mathrm{QM}}(\vec{a}, \vec{b}) = \cos[2(\theta_a - \theta_b)], \tag{1.138}$$

hence

$$S_{AB}^{\mathrm{QM}} = \cos[2(\theta_a - \theta_b)] - \cos[2(\theta_a - \theta_{b'})] + \cos[2(\theta_{a'} - \theta_b)] + \cos[2(\theta_{a'} - \theta_{b'})]. \tag{1.139}$$

There exists particular sets of angles making this function violates the CHSH inequality.

To systematically determine the parameter space violating the CHSH inequality, let's denote

$$\theta_1 = \theta_a - \theta_b, \quad \theta_2 = \theta_{a'} - \theta_{b'}, \quad \theta_3 = \theta_{a'} - \theta_b, \tag{1.140}$$

then

$$S_{AB}^{\mathrm{QM}} = \cos(2\theta_a) - \cos[2(\theta_1 + \theta_2 + \theta_3)] + \cos(2\theta_2) + \cos(2\theta_3). \tag{1.141}$$

This is symmetric for θ_1, θ_2 and θ_3, and the extreme condition is

$$\sin\alpha - \sin 3\alpha = 0, \quad \theta_1 = \theta_2 = \theta_3 = \frac{\alpha}{2}. \tag{1.142}$$

Hence $\alpha = 0, \pm\pi, \pm\pi/4, \pm 3\pi/4$. The corresponding exterme values are

$$S_{AB}^{\mathrm{QM}}(\alpha) = 3\cos\alpha - \cos 3\alpha \in \{\pm 2, \pm 2\sqrt{2}\}. \tag{1.143}$$

The CHSH inequality can be stated more generally for a bipartite system, one part of which is measured by Alice while the other is measured by Bob. Alice can measure one of the two observables A and A', while Bob measures B and B'. We assume their values are confined in ± 1, and are all functions of local hidden variables. We again have

$$\sigma_{AB}(\lambda) \equiv A(B - B') + A'(B + B') \in \pm 2, \tag{1.144}$$

hence

$$\langle \sigma_{AB} \rangle_\lambda \equiv \int \mathrm{d}\lambda \ \rho(\lambda) \sigma_{AB}(\lambda) \in [-2, 2], \tag{1.145}$$

$$-2 \leq \langle AB \rangle - \langle A'B \rangle + \langle AB' \rangle + \langle A'B' \rangle \leq 2. \tag{1.146}$$

Let the observables A, A', B, B' be the spins measured along different drections, then the

quantum expectation values are

$$\langle \Psi_B | \vec{\sigma}_a \cdot \vec{\sigma}_b | \Psi_B \rangle = -\vec{a} \cdot \vec{b}, \tag{1.147}$$

where $|\Psi_B\rangle$ is the Bell's state. We find the case

$$\vec{a} = \hat{y}, \quad \vec{a}' = \hat{x}, \quad \vec{b} = \frac{-\hat{x} + \hat{y}}{\sqrt{2}}, \quad \vec{b}' = \frac{\hat{x} + \hat{y}}{\sqrt{2}} \tag{1.148}$$

violates the CHSH inequality.

1.2.8 Bell Inequalities and Entanglement

Let's consider a separable pure state $|AB\rangle = |A\rangle \otimes |B\rangle$, the

$$\langle AB \rangle = \mathrm{Tr}(AB) = \langle A \rangle \langle B \rangle . \tag{1.149}$$

It's always possible to construct a hidden-variable theory reproduces the results of quantum mechanics for a single qubit, hence, no violation of Bell-like inequalities can occur in the separable case.

For a general entangled state for two qubits, any such state can be written in aa Schmidt basis such that

$$|\psi\rangle = \alpha |1\rangle + \beta |-1\rangle . \tag{1.150}$$

We can always make $\alpha, \beta \in \mathbb{R}^+$. Besides, we cal always orient the coordinate frame making $|\pm 1\rangle$ eigenstates of $\sigma_z \otimes \sigma_z$. Now Alice and Bob measure the spin in the xz-plane, hence

$$\sigma_A = \sigma_x \sin\theta_A + \sigma_z \cos\theta_A, \quad \sigma_B = \sigma_x \sin\theta_B + \sigma_y \cos\theta_B, \tag{1.151}$$

then

$$\langle \psi | \sigma_A \otimes \sigma_B | \psi \rangle = 2\alpha\beta \sin\theta_A \sin\theta_B + \cos\theta_A \cos\theta_B. \tag{1.152}$$

The result for a Bell's state is revocered for $\alpha = \beta = 1/\sqrt{2}$, and we can actually show any entangled state whose $\alpha\beta \neq 0$ violates the CHSH inequality. We choose $\theta_A = -\theta'_A$, $\theta_B = 0$, $\theta'_B = \pi/2$, hence the CHSH ineqquality demands

$$-1 \leq \cos\theta - 2\alpha\beta \sin\theta \leq 1, \tag{1.153}$$

but this could be violated since

$$\cos\theta - 2\alpha\beta \sin\theta = \sqrt{1 + 4\alpha^2\beta^2} \cos\left(\theta + \arcsin \frac{2\alpha\beta}{\sqrt{1 + 4\alpha^2\beta^2}}\right), \quad \sqrt{1 + 4\alpha^2\beta^2} > 1. \tag{1.154}$$

1.2.9 No Cloning Theorem

Suppose we have an operator $U : |0\rangle_A \otimes |\phi\rangle_B \mapsto |0\rangle_A \otimes |0\rangle_B$, $|1\rangle_A \otimes |\phi\rangle_B \mapsto |1\rangle_A \otimes |1\rangle_B$, which means the operators make the system B copy the state of system A. Suppose Alice

prepares a general state

$$|\psi\rangle = a\,|0\rangle_A + b\,|1\rangle_B\,, \tag{1.155}$$

then

$$U(|\psi\rangle_A \otimes |\phi\rangle_B) = a\,|0\rangle_A \otimes |0\rangle_B + b\,|1\rangle_A \otimes |1\rangle_B \neq |\psi\rangle_A \otimes |\psi\rangle_B\,. \tag{1.156}$$

Hence, a general state cannot be copied even if the operator U can copy the basis states spanning the state.

1.3 Quantum Information

1.3.1 Principles of a Quantum Computer

A classical computer has n bits with 2^n possible outputs, while a quantum computer has n qubits with ∞ possible outcomes. A quantum computer's calculation is probablistic, and several projections are necessary to obtain the full answers.

Consider a quantum computer with n quibits, a quantum computer calculation consists of initializing all the qubits to $|0\rangle$ and applying a unitary evolution U. At the end of computation, the set of qubits is projected and a register of classical bits is retrived from the system:

$$|\mathbf{0}\rangle \equiv \bigotimes_{i=1}^{N} |0\rangle \mapsto U\,|\mathbf{0}\rangle = \sum_{\{\sigma_i\}} C_{\sigma_1 \cdots \sigma_N} \bigotimes_{i=1}^{N} |\sigma_i\rangle\,. \tag{1.157}$$

The Hilbert space of n qubits has dimension 2^n, hence 2^n calculations are parallelly executed at the same time (with the help of Hadamard gates).

Errors are inevitable in such a probablistic computation pipline. Define $f_i \in (0,1)$ as the fidelity of the gate i representing the correctness of a computation unit, then an m-gate system has fidelity $\prod_{i=1}^{m} f_i$. Therefore, there's a competition between the parallelness and the errors, and quantum error correction is an indespensible part of a quantum computer.

A toy model for computation focuses on the addtion $\oplus : \{0,1\} \times \{0,1\} \to \{0,1\}$ defined as

$$a \oplus b = (a + b) \mod 2. \tag{1.158}$$

To implement this computation on aa quantum circuit, we have to use the Hadamard gaate

$$U_H \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{1.159}$$

then

$$U_H \otimes \mathbb{1}\,|0\rangle \otimes |0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle\,. \tag{1.160}$$

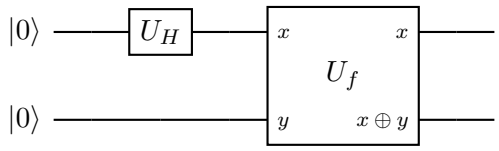
Now we can define the operator U_f for f evaluation such that

$$U_f\,|x\rangle \otimes |y\rangle = |x\rangle \otimes |x \oplus y\rangle\,, \tag{1.161}$$

then we have

$$U_f(U_H \otimes \mathbb{1})\,|0\rangle \otimes |0\rangle = \frac{1}{\sqrt{2}}(|1\rangle \otimes |f(0,0)\rangle + |1\rangle \otimes |f(1,0)\rangle). \tag{1.162}$$

Therefore, two calculations for f are obtained at the same time. Since we are using unitary operators for computation, hence it's reversible. In contrary, a classical computation is not.



1.4 Single Qubit Gates

Logic gates of qubits can be thought of as rotations on the Bloch sphere, and any single unitary operator can be written as

$$U = e^{\mathrm{i}\phi} R_{\hat{n}}(\alpha). \tag{1.163}$$

Three basic gates are the Pauli matrices:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{1.164}$$

$$Y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \tag{1.165}$$

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.166}$$

The Hadamard gate writes

$$H = \frac{1}{\sqrt{2}}(X + Z) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{1.167}$$

A $\pi/2$-rotation along the 3-axis is conventionally called a phase S, which reads

$$S = \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{i} \end{pmatrix}, \tag{1.168}$$

while a $\pi/4$-rotation along the 3-axis is called T,

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{\mathrm{i}\pi/4} \end{pmatrix}. \tag{1.169}$$

Any unitary qubit operator can be writtes as

$$U(\alpha,\beta,\gamma,\delta) = e^{\mathrm{i}\alpha} R_Z(\beta) R_Y(\gamma) R_Z(\delta). \tag{1.170}$$

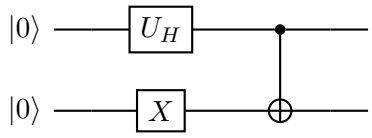
The proof starts with noticing U can always be diagonalized.

1.5 Two Qubit Gates

The most important two qubit gate is the CNOT (control-not) gate:

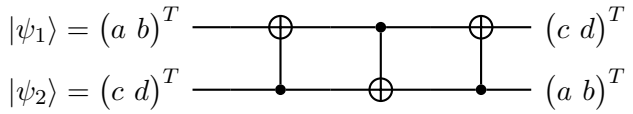
$$\mathbf{CNOT} = \begin{pmatrix} \mathbb{1}_{2\times 2} & 0 \\ 0 & \mathbf{X} \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{1.171}$$

It flips the second qubit if the first qubit is $|1\rangle$, and it does nothing if the first qubit is $|0\rangle$. The Bell's state $|\Phi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ can be replaced by The vertial line represents a

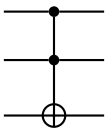


CNOT gate.

A theorem states that the CNOT gate and single qubit states form a universial set for any multiple qubit system. Besides, the CNOT gate can relize teleportation by



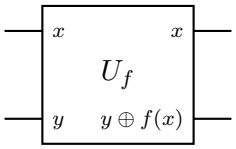
The CNOT gate can be generalized to 3-qubit gates by defining the third qubit is flipped if the first two states are $|1\rangle$ otherwise nothing happens. This is called the Toffoli gate and can be represented as

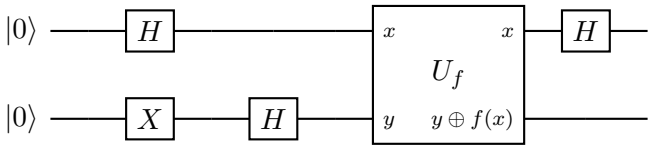


1.6 Quantum Algorithm

1.6.1 The Deutsch Algorithm

Consider the following unitary transformation
where $f : \{0,1\} \to \{0,1\}$ is some unknown function and $\oplus$ is the plus modulo two. For a classical computer, we have to compute $f(0)$ and $f(1)$ respectively to determine if $f(1) = f(0)$, but a quantum computer only needs to compute once via the following circuit:



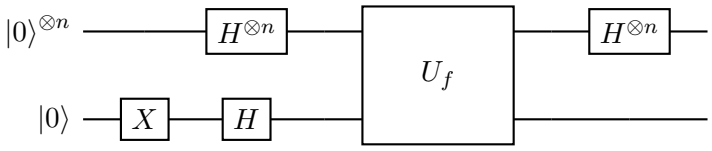


The output state is

$$|\psi_o\rangle = (H \otimes \mathbb{1}) U_f (\mathbb{1} \otimes H)(H \otimes X) |0\rangle \otimes |0\rangle , \tag{1.172}$$

we find if the x part of $|\psi_o\rangle$ is 1, then $f(1) = f(0)$; while $f(1) \neq f(0)$ corresponds to the output $x = 0$.

The Deutsch algotirhm can be generalized to a system of n qubits and giving the Deutsch-Josza algorithm. Here we consider a function $f(\boldsymbol{x})$ defined for a configuration of qubits, it is either constant for all $\{x_i\}$ or balanced in the sense that for half of the qubit states configurations we have $f(\boldsymbol{x}) = 0$, while for the half we have $f(\boldsymbol{x}) = 1$. A classical answer demands us to measure $f(\boldsymbol{x})$ for $2^{n-1} + 1$ qubits, but the quantum answer only needs the following circuit:



The input writes $|\psi_i\rangle = |0\rangle \otimes |0\rangle^{\otimes n}$, then

$$|\psi_1\rangle = (H \otimes \mathbb{1})(X \otimes \mathbb{1})(\mathbb{1} \otimes H^{\otimes n}) |\psi_i\rangle = \frac{1}{\sqrt{2^n}} \sum_{\{x_i\}} \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \otimes |\boldsymbol{x}\rangle . \tag{1.173}$$

After the action of U_f, there should be

$$|\psi_2\rangle = U_f |\psi_1\rangle = \frac{1}{\sqrt{2^n}} \sum_{\{x_i\}} (-1)^{f(\boldsymbol{x})} (|0\rangle - |1\rangle) \otimes |x\rangle . \tag{1.174}$$

Since a Hadamard gate acts like

$$H |x\rangle = \frac{1}{\sqrt{2}} \sum_z (-1)^{xz} |z\rangle , \tag{1.175}$$

we have

$$H^{\otimes n}\left|\boldsymbol{x}\right\rangle = \frac{1}{\sqrt{2^n}}\sum_{\{z_i\}}(-1)^{\boldsymbol{x}\cdot\boldsymbol{z}}\left|\boldsymbol{z}\right\rangle. \tag{1.176}$$

The final output then writes

$$\left|\psi_o\right\rangle = \frac{1}{2^n}\sum_{\{x_i\},\{z_i\}}(-1)^{\boldsymbol{x}\cdot\boldsymbol{z}+f(\boldsymbol{x})}(\left|0\right\rangle - \left|1\right\rangle)\otimes\left|\boldsymbol{z}\right\rangle. \tag{1.177}$$

We can consider projecting $\left|\psi_o\right\rangle$ onto the state $\left|\boldsymbol{z}=\boldsymbol{0}\right\rangle$, then we have the state

$$\frac{1}{2^n}\sum_{\{x_i\}}(-1)^{f(\boldsymbol{x})}(\left|0\right\rangle - \left|1\right\rangle). \tag{1.178}$$

If f is constant, we find a non-zero state; while if f is balanced, we have zero. Therefore, classically $2^{n-1}+1$ measurements can be replaced by a single one measurement.

1.7 Mixed States and the Bloch Sphere

The density matrix of a single qubit has 3 independent degrees of freedom and a normalized trace, and can always be written as

$$\rho = \frac{1}{2}(\mathbb{1} + \hat{n}\cdot\boldsymbol{\sigma}), \tag{1.179}$$

$\hat{n}\in\mathbb{R}^3$ is called the Bloch vector, and ρ can be thought of as a point in the interior of the Bloch sphere given by $|\hat{n}|$.

If ρ is a pure state, then $\hat{n}$ is of unit length, hence it locates on the usual Bloch sphere; while if ρ is a maximally mixed state, we have $\hat{n}=0$, other cases fall somewhere in between.

Now let's cosider decoherence via entanglement. For an isolated qubit A, it follows a unitary evolution keeping it in pure state and $\det\rho = 0$. However, if this qubit is coupled to the environment with entanglement, the reduced density matrix of the subsystem will evolves to a mixed state.

A nontrivial converse is that for any maixed state ρ_A, we can find an entangled pure state for the Hilbert space for A coupling to another sytem, which is called the "purification".

The proof starts with the Schmidt decomposed form of ρ_A:

$$\rho_A = \sum_i p_i\left|i\right\rangle\!\left\langle i\right|. \tag{1.180}$$

The system B is chosen to have the same Hilbert space as A, and we can define a pure state for $\mathscr{H}_A\otimes\mathscr{H}_B$ s.t.

$$\left|A\otimes B\right\rangle = \sum_i\sqrt{p_i}\left|i\right\rangle\otimes\left|i\right\rangle, \tag{1.181}$$

then

$$\rho_{A\otimes B} = \sum_{i,j}\sqrt{p_ip_j}\left|i;i\right\rangle\!\left\langle j;j\right|. \tag{1.182}$$

Clearly

$$\rho_A = \mathrm{tr}_B\, \rho_{A\otimes B} = \sum_i p_i \left|i\right\rangle\!\left\langle i\right| . \tag{1.183}$$

Of course, such purification is not unique.

1.8 Quantum Channels

This is a general formalism describing the evolution of systems coupled to the environment. For an open system A coupled with B, we can consider the total syatem $A\otimes B$ as an isolated closed system. Now the evolution for ρ_A is no longer unitary, but is given by

$$\mathcal{E}(\rho_A) = \mathrm{tr}_B[U_{AB}(t)\rho_{A\otimes B}(0)U_{AB}^\dagger(t)]. \tag{1.184}$$

We can always take the state for B at $t = 0$ to be a pure state $\rho_B = |\psi_B\rangle\langle\psi_B|$ without a loss of geenrality, then we find

$$\mathcal{E}(\rho_A) = \sum_k \left\langle \psi_B^{(k)} \middle| U(t)(\rho_A \otimes |\psi_B\rangle\langle\psi_B|)U^\dagger(t) \middle| \psi_B^{(k)} \right\rangle \equiv \sum_k M_k \rho_A M_k^\dagger. \tag{1.185}$$

Here M_k are called the Krauss operators which are not unitary.

For a concrete example, consider a qubit system coupling with the environment given by a qubit, then any two-qubit operator can be written on the 4-dimensional Hilbert space spanned by $\{|00\rangle, |10\rangle, |01\rangle, |11\rangle\}$. The the unitary evolution operator is characterized as

$$U = \begin{pmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{pmatrix}, \quad U_{ij} = \langle i|U|j\rangle_B . \tag{1.186}$$

In this case, denote

$$U = U_{\mu\nu;\rho\sigma} \left|\mu\right\rangle\!\left\langle\nu\right|_A \otimes \left|\rho\right\rangle\!\left\langle\sigma\right|_B , \tag{1.187}$$

Then

$$\begin{aligned} \mathcal{E}(\rho_A) &= \sum_k \langle k, B|U_{\mu\nu;\rho\sigma} \left|\mu\right\rangle\!\left\langle\nu\right|_A \otimes \left|\rho\right\rangle\!\left\langle\sigma\right|_B (\rho_A \otimes |\psi\rangle\langle\psi|_B) U^*_{\mu'\nu';\rho'\sigma'} \left|\nu'\right\rangle\!\left\langle\mu'\right|_A \otimes \left|\sigma'\right\rangle\!\left\langle\rho'\right|_B |k, B\rangle \\ &= \sum_k U_{\mu\nu;k\sigma} U^*_{\mu'\nu';k\sigma'} \left|\mu\right\rangle\!\left\langle\nu\right|_A \rho_A \left|\nu'\right\rangle\!\left\langle\mu'\right|_A \langle\sigma|\psi\rangle_B \left\langle\psi|\sigma'\right\rangle_B . \end{aligned} \tag{1.188}$$

Define

$$M_k = U_{\mu\nu;k\sigma} \langle\sigma|\psi\rangle_B \left|\mu\right\rangle\!\left\langle\nu\right|_A , \tag{1.189}$$

we find

$$\mathcal{E}(\rho_A) = \sum_k M_k \rho_A M_k^\dagger. \tag{1.190}$$

Since U is unitary, we have

$$\sum_k \langle k|UU^\dagger|k\rangle = \mathbb{1}_A, \tag{1.191}$$

hence

$$\sum_k M_k M_k^\dagger = \mathbb{1}_A, \tag{1.192}$$

which is a key sum-rule for Krauss matrices. It's essential for keeping $\mathrm{tr}[\mathcal{E}(\rho_A)]$ normalized.

Another key point for $\mathcal{E}(\rho_A)$ to be a valid density matrix is the positive-definiteness, i.e., $\forall\, |a\rangle \in \mathscr{H}_A$, we expect

$$\sum_k \langle a|M_k \rho_A M_k^\dagger|a\rangle \geq 0. \tag{1.193}$$

This is true since we can insert in the Schmidt decomposed form of ρ_A,

$$\rho_A = \sum_i p_i \,|i\rangle\langle i|\,, \tag{1.194}$$

then

$$\langle a|\mathcal{E}(\rho_A)|a\rangle = \sum_i p_i \sum_k |\,\langle a|M_k|i\rangle\,|^2 \geq 0. \tag{1.195}$$

We conclude that $\mathcal{E} : \rho_A \mapsto \rho'_A$ is a positive trace-preserving (or rather, completely positive trace-preserving) map. Besides, $\mathcal{E}$ is reversible only if it's unitary. According to the Stinespring dialation, for any $\mathscr{E}$-evolution, we can alyways construct an environment coupled to the open system such that the whole system evolves according to a unitary operator U.

Now we enumerate some quantum channels:

1. Amplitude damping channel: Physically, it corresponds to a qubit decaying from $|1\rangle$ to $|0\rangle$, emitting a photon to the environment. (Needs the Markovian assumption that no back reaction from the environment.)

   Here the unitary evolution operator for the whole system acts like

   $$|0\rangle \otimes |0\rangle \to |0\rangle \otimes |0\rangle\,, \quad |1\rangle \otimes |0\rangle \to \sqrt{1-p}\,|1\rangle \otimes |0\rangle + \sqrt{p}\,|0\rangle \otimes |0\rangle\,. \tag{1.196}$$

   The Krauss operators then acts like

   $$M_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 0 \\ \sqrt{p} & 0 \end{pmatrix}. \tag{1.197}$$

   Consider a general density matrix

   $$\rho_A = \begin{pmatrix} a & be^{\mathrm{i}\beta} \\ be^{-\mathrm{i}\beta} & 1-a \end{pmatrix}, \tag{1.198}$$

   then the $\mathcal{E}$-evolution reads

   $$\mathcal{E}[\rho_A] = \begin{pmatrix} a + p(1-a) & be^{\mathrm{i}\beta}\sqrt{1-p} \\ be^{-\mathrm{i}\beta}\sqrt{1-p} & (1-a)(1-p) \end{pmatrix}. \tag{1.199}$$

The larger p, the smaller the off-diagonal components and the $|1\rangle\langle 1|$-element, the larger the $|0\rangle\langle 0|$-element.

2. Dephasing (phase-damping) channel: Physically, the environment scatters off the qubit into a higher state, where the total unitary evolution reads

$$|0\rangle \otimes |0\rangle \to \sqrt{1-p}\,|0\rangle \otimes |0\rangle + \sqrt{p}\,|0\rangle \otimes |1\rangle\,, \tag{1.200}$$
$$|1\rangle \otimes |0\rangle \to \sqrt{1-p}\,|1\rangle \otimes |0\rangle + \sqrt{p}\,|1\rangle \otimes |2\rangle\,. \tag{1.201}$$

The Karuss matrices are

$$M_0 = \sqrt{1-p}\mathbb{1}, \quad M_1 = \begin{pmatrix} \sqrt{p} & 0 \\ 0 & 0 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix}. \tag{1.202}$$

Then

$$\mathcal{E}[\rho_A] = \begin{pmatrix} a & (1-p)be^{\mathrm{i}\beta} \\ (1-p)be^{-\mathrm{i}\beta} & 1-a \end{pmatrix}. \tag{1.203}$$

3. Depolarizing channel: The spins in the system is flipped by the action of Pauli matrices[1]The unitary evolution writes

$$|\psi\rangle \otimes |0\rangle \to \sqrt{1-p}\,|\psi\rangle \otimes |0\rangle + \sum_{i=1}^{3} \sqrt{\frac{p}{3}}\sigma_i\,|\psi\rangle \otimes |i\rangle\,. \tag{1.204}$$

The four Krauss operators are

$$M_0 = \sqrt{1-p}\mathbb{1}, \quad M_i = \frac{\sqrt{p}}{3}\sigma_i. \tag{1.205}$$

Then the $\mathcal{E}$-evolution is

$$\mathcal{E}[\rho_A] = \frac{2}{3}p\mathbb{1} + \left(1 - \frac{4p}{3}\right)\rho_A. \tag{1.206}$$

1.9 From von Neumann to Lindblad

The time evolution of a closed system is given by the unitary evolution

$$\partial_t \rho = -\frac{\mathrm{i}}{\hbar}[H, \rho]. \tag{1.207}$$

Once the system is open, we expect some additional non-unitary terms breaking the unitary evolution and bringing decoherence. Suppose the non-unitarity is opened at time t, then

$$\rho(t + \mathrm{d}t) = \mathcal{E}[\rho(t)] = \sum_{\alpha} M_\alpha(\mathrm{d}t)\rho(t)M_\alpha^\dagger(\mathrm{d}t). \tag{1.208}$$

[1] σ_x is called the bit-flip operator, σ_z is phase flipping, σ_y is bit-phase flipping.

The ansatz for the Krauss operators reads

$$M_0 = \mathbb{1} + (K - \mathrm{i}H/\hbar)\mathrm{d}t, \quad M_k = \sqrt{\gamma_k \mathrm{d}t} L_k, \tag{1.209}$$

where K and H are Hermitian. The sum-rule for the Krauss operators demands

$$\mathbb{1} = \sum_\alpha M_\alpha M_\alpha^\dagger \;\Rightarrow\; K = -\frac{1}{2}\sum_{k>0} \gamma_k L_k^\dagger L_k. \tag{1.210}$$

Hence

$$\frac{\partial \rho}{\partial t} = -\frac{\mathrm{i}}{\hbar}[H, \rho] - \frac{1}{2}\sum_{k>0}\gamma_k \{L_k^\dagger L_k, \rho\} + \sum_{k>0}\gamma_k L_k \rho L_k^\dagger, \tag{1.211}$$

which is called the Lindblad master equation.

2 Mesoscopic Quantum Transport and Superconductivity

The Drude model is the simplest model for explaining the resistence in metals, where we assume electrons randomly collide with lattices/impurities, and the average time between two collisions is denoted as τ. Then the momentum of an electron at $t + \mathrm{d}t$ reads

$$\boldsymbol{p}(t + \mathrm{d}t) = \frac{\mathrm{d}t}{\tau}\boldsymbol{p}_{\text{random}} + \left(1 - \frac{\mathrm{d}t}{\tau}\right)[\boldsymbol{p}(t) + \boldsymbol{F}\mathrm{d}t]. \tag{2.1}$$

Taking the expectation value and we find

$$\frac{\partial \boldsymbol{p}}{\partial t} = -\frac{1}{\tau}\boldsymbol{p} + \boldsymbol{F}, \tag{2.2}$$

and the steady state have

$$\boldsymbol{p} = \tau \boldsymbol{F}. \tag{2.3}$$

Driven by electric field $\boldsymbol{E}$, $\boldsymbol{F} = -e\boldsymbol{E}$, and $\boldsymbol{j} = -en(\mathcal{E}_F)\boldsymbol{p}/m_e$, hence we find

$$\boldsymbol{j} = \frac{1}{m_e} n(\mathcal{E}_F)\tau e^2 \boldsymbol{E}, \tag{2.4}$$

and the Drude conductivity reads

$$\sigma = \frac{n(\mathcal{E}_F)\tau e^2}{m_e}, \tag{2.5}$$

and the conductivity is given by

$$I = GV, \qquad G = \frac{\sigma S}{L}. \tag{2.6}$$

This result only valides when there's no quantum coherence and τ is way smaller than the characteristic time for the charge carrier to move in the experiment.

Now our task is to formulate a quantum transport theory for cases wher the Drude's

approach no longer valides. The Landauer approach directly computes the conductance of a mesoscopic system. Such a mesoscopic set-up usually contains three parts:

- The contact (resrvoirs): They are big ($\sim$ mm) metallic pads with a given temperature T and the electrochemical potential μ, within which the electrons follow the F-D distribution
$$f(E) = \frac{1}{e^{\frac{1}{k_B T}(E-\mu)} + 1}. \tag{2.7}$$
A well-defined T and μ also implies the non-existence of quantum coherence here.
- The leads: They are perfect metallic wire connecting the reservoirs to the sample.
- The sample: It could contain disorders causing the scattering centers, and it's usually quantum coherent.

Therefore, we have to establish a quantum theory for the transport in the leads and in the sample respectively.

2.1 The Conductance of a Perfect Wire

The lead can be modelled as a box (L_x, L_y, L_z) with $L_z \gg L_x, L_y$, and for electrons in it we take the simplest confining potential

$$V(x,y) = \begin{cases} 0, & 0 \le x, y \le L_x, L_y, \\ +\infty, & \text{otherwise.} \end{cases} \tag{2.8}$$

Clearly, the eigenstate for the Schrödinger equation

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi + V(x,y)\psi = \mathcal{E}\psi \tag{2.9}$$

is given by

$$\psi_{n_x,n_y,k_z}(x,y,z) = \frac{2}{\sqrt{L_x L_y L_z}} e^{\mathrm{i}k_z z} \sin\frac{n_x \pi x}{L_x} \sin\frac{n_y \pi y}{L_y} \equiv \frac{1}{\sqrt{L_z}} e^{\mathrm{i}k_z z} \chi_{n_x,n_y}(x,y), \tag{2.10}$$

with the energy

$$\mathcal{E}(n_x, n_y, k_z) = \frac{\hbar^2}{2m_e}\left(k_z^2 + \frac{n_x^2\pi^2}{L_x^2} + \frac{n_y^2\pi^2}{L_y^2}\right). \tag{2.11}$$

Each horizontal eigenstate (n_x, n_y) is called a conduction/transmission channel.

Given a state ψ, the current density associated to it reads

$$\boldsymbol{j} = \frac{e\hbar}{m}\,\mathrm{Im}(\psi^*\nabla\psi), \tag{2.12}$$

and the current flowing through it is given by

$$I = \int \mathrm{d}x\mathrm{d}y\; j_z(x,y). \tag{2.13}$$

For the perfect wire eigenstate ψ_{n_x,n_y,k_z}, we find

$$j_z^{(n_x,n_y,k_z)} = \frac{4e\hbar}{mL_xL_yL_z} k_z \sin^2\frac{n_x\pi x}{L_x}\sin^2\frac{n_y\pi y}{L_y}, \tag{2.14}$$

$$i_{(n_x,n_y,k_z)} = \frac{e\hbar}{mL_z}k_z. \tag{2.15}$$

Right-moving states with $k_z > 0$ are injected from the left reservoir whose electron sate occupation is given by the F.D. distribution with μ_L, while left-movers are injected from the right reservoir with μ_R. Then the left-to-right current with horizontal mode (n_x, n_y) is

$$I_{L\to R}^{(n_x,n_y)} = \sum_{k>0} f(k,\mu_L) i_{(n_x,n_y,k)}. \tag{2.16}$$

In 1D continuum limit, we have

$$\rho_1(\varepsilon)\mathrm{d}\varepsilon = \frac{2L_z}{\pi}\mathrm{d}k \;\Rightarrow\; \rho_1(\varepsilon) = \frac{2L_z}{\pi\hbar v(\varepsilon)}, \tag{2.17}$$

where

$$v(\varepsilon) = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial k} = \frac{\hbar k}{m}, \tag{2.18}$$

and we can rewrite the current in terms of an integral over the energy:

$$\begin{aligned} I_{L\to R}^{(n_x,n_y)} &= \frac{1}{2}\int \mathrm{d}\varepsilon\; \rho_1(\varepsilon)\vartheta[\varepsilon - \mathcal{E}(n_x,n_y,0)] f(\varepsilon,\mu_L) i_{(n_x,n_y,k)} \\ &= \frac{L_z}{\pi\hbar}\int \mathrm{d}\varepsilon\; \vartheta[\varepsilon - \mathcal{E}(n_x,n_y,0)] f(\varepsilon,\mu_L)\frac{e}{L_z} \\ &= \frac{e}{\pi\hbar}\int \mathrm{d}\varepsilon\; \vartheta[\varepsilon - \mathcal{E}(n_x,n_y,0)] f(\varepsilon,\mu_L). \end{aligned} \tag{2.19}$$

The net current carried by the (n_x, n_y)-channel then reads

$$I_{(n_x,n_y)} = I_{L\to R}^{(n_x,n_y)} - I_{R\to L}^{(n_x,n_y)} = \frac{2e}{h}\int \mathrm{d}\varepsilon\; \vartheta[\varepsilon - \mathcal{E}(n_x,n_y,0)][f(\varepsilon,\mu_L) - f(\varepsilon,\mu_R)], \tag{2.20}$$

and the total current is

$$I_{\text{total}} = \frac{2e}{h}\sum_{n_x,n_y}\int \mathrm{d}\varepsilon\; \vartheta[\varepsilon - \mathcal{E}(n_x,n_y,0)][f(\varepsilon,\mu_L) - f(\varepsilon,\mu_R)]. \tag{2.21}$$

This is the Landauer formula.

Let's define

$$M(\varepsilon) \equiv \sum_{n_x,n_y} \vartheta[\varepsilon_F - \mathcal{E}(n_x,n_y,0)]. \tag{2.22}$$

$M(\varepsilon_F)$ roughly counts the number of propagating modes in the wire.

$$M(\varepsilon_F) = \frac{L_xL_y}{(\lambda_F/2)^2} = \frac{Sk_F^2}{\pi^2} = \frac{2m_eS}{\pi^2\hbar^2}\varepsilon_F. \tag{2.23}$$

In general $\mu_L - \mu_R = eV$ is way smaller than the energy spacing between two nearby channels, hence $M(\varepsilon) = M(\varepsilon_F)$ and

$$I = \frac{2e}{h} M(\varepsilon_F) \int \mathrm{d}\varepsilon \, [f(\varepsilon, \mu_L) - f(\varepsilon, \mu_R)]. \tag{2.24}$$

At $T = 0$, it directly gives

$$I = \frac{2e^2 V}{h} M(\varepsilon_F) \tag{2.25}$$

for small V, hence the conductance reads

$$G = \frac{I}{V} = \frac{2e^2}{h} M(\varepsilon_F). \tag{2.26}$$

This inspires us to define the conduntance quantum

$$G_Q \equiv \frac{2e^2}{h}, \quad R_Q = 1/G_Q \approx 13 \text{ k}\Omega. \tag{2.27}$$

Note even though the wire is modeled to be perfect, the existence of a finite conductance still implies the existence of dissipation. Here the dissipation hides in the reservoirs for maintaining a fixed T and μ requires energy relaxiation.

Electrons in the perfect wire are out-of-equilibrium, but we still could talk about the probability finding an electrom at energy $\mathcal{E}$. Since electrons with $k > 0$ follow $f(\mathcal{E}, \mu_L)$, those $k < 0$ follow $f(\mathcal{E}, \mu_R)$, we intuitively expect

$$P(\mathcal{E}) = \frac{1}{2}[f(\mathcal{E}, \mu_L) + f(\mathcal{E}, \mu_R)]. \tag{2.28}$$

Clearly, for more general case it should be written as

$$P(\mathcal{E}) = P(\mathcal{E}|k > 0)P(k > 0) + P(\mathcal{E}|k < 0)P(k < 0). \tag{2.29}$$

Although the chemical potential for the electrons in the wire is ill-defined, we can nevertheless define μ^* to be the chemical potential would appear if the electrons in the wire are thermalized, i.e.

$$\int \mathrm{d}\varepsilon \, \rho_1(\varepsilon) P(\varepsilon) \equiv \int \mathrm{d}\varepsilon \rho_1(\varepsilon) f(\varepsilon, \mu^*). \tag{2.30}$$

For $T = 0$ and constant $\rho_1(\varepsilon)$, one find

$$\mu^* = \frac{\mu_L + \mu_R}{2}, \tag{2.31}$$

and there are potential drops of $eV/2$ at the contacts between the wire and the reservoirs.

We can also consider two points A, B within the wire and think about the inrtinsic conductance of the wire. Since μ^* is constant along the wire, we find $\Delta\mu_{AB} = 0$, hence $G_{\text{intrinsic}} = \infty$. It's consistent with our assumption that there is no scattering in the wire, and the previously computed conductance is purly contact conductance.

2.2 Quasi 1D Wire with Disorder

Single-Channel: We start from the toy model of a pure 1D lead with a single impurity lying in it, which can be modelled as a single interface with transmission amplitude $t(k)$ and reflection amp $r(k)$. For a single injected right-moving sigenstate $\psi_i = \frac{1}{\sqrt{L_z}} e^{\mathrm{i}k_z}$, the transmitted wavefunction is $\psi_t = t\psi_i$, while the reflected one is $\psi_r = r\psi_i$. Therefore, the right-moving current is

$$i_{L\to R}(k) = \frac{e\hbar}{mL_z}|t(k)|^2 k. \tag{2.32}$$

The total right-flowing current then reads

$$I_{L\to R} = \frac{1}{2}\int \mathrm{d}\varepsilon\ \rho_1(\varepsilon) i_{L\to R}[k(\varepsilon)] f(\varepsilon,\mu_L) = \frac{2e}{h}\int \mathrm{d}\varepsilon\ T(\varepsilon) f(\varepsilon,\mu_L), \tag{2.33}$$

where we denote $T(\varepsilon) \equiv |t(\varepsilon)|^2$. Similarly, the left-moving current is

$$I_{R\to L} = \frac{2e}{h}\int \mathrm{d}\varepsilon\ T'(\varepsilon) f(\varepsilon,\mu_R). \tag{2.34}$$

A priori $T \neq T'$, but $\mu_L = \mu_R \ \Rightarrow\ I = 0$ imposes $T = T'$, hence the total current reads

$$I = \frac{2e}{h}\int \mathrm{d}\varepsilon\ T(\varepsilon)[f(\varepsilon,\mu_L) - f(\varepsilon,\mu_R)] = \frac{2e^2}{h} T(\varepsilon) V. \tag{2.35}$$

At $T = 0$, we find

$$G = \frac{2e^2}{h} T(\varepsilon_F). \tag{2.36}$$

Now we can talk about the intrinsic resistance of the wire between two points A, B located at opposite sides (A left, B right) of the impurity. Now we have

$$P_A(\varepsilon|k>0) = f(\varepsilon,\mu_L), \tag{2.37}$$
$$P_A(\varepsilon|k<0) = Rf(\varepsilon,\mu_L) + Tf(\varepsilon,\mu_R), \tag{2.38}$$

and

$$P_A(k>0) = P_A(k<0) = \frac{1}{2}, \tag{2.39}$$

hence

$$P_A(\varepsilon) = \frac{1}{2}[(1+R)f(\varepsilon,\mu_L) + Tf(\varepsilon,\mu_R)], \tag{2.40}$$

likewise

$$P_B(\varepsilon) = \frac{1}{2}[Tf(\varepsilon,\mu_L) + (1+R)f(\varepsilon,\mu_R)]. \tag{2.41}$$

We can again define the effecitve chemical potential for P_A and P_B, and at $T = 0$ with constant ρ_1 we find

$$\mu_A^* = \frac{1}{2}(1+R)\mu_L + \frac{1}{2}T\mu_R, \quad \mu_B^* = \frac{1}{2}T\mu_L + \frac{1}{2}(1+R)\mu_R. \tag{2.42}$$

Note $R = 1 - T$, then

$$\Delta\mu^*_{AB} = (1-T)(\mu_L - \mu_R) = (1-T)eV. \tag{2.43}$$

Hence we can define the intrinsic resistance as

$$R_{\rm int} \equiv \frac{\Delta\mu^*_{AB}}{eI} = \frac{h}{2e^2}\frac{1-T}{T} = R_Q\frac{1-T}{T}. \tag{2.44}$$

Note

$$R_{\rm tot} = R_{\rm int} + 2\times\frac{1}{2}R_Q, \tag{2.45}$$

we can interpret it as the total resistance is the intrinsic resistance of the single impurity plus the two contact resistance at the two reservoirs in serial. For a M-channel case the total contact resistance will be reduced to R_Q/M.

Multi-Channel: Once we introduce more channels, the presence of the impurity may scatter a mode to different channels. For simplicity, we considier a 2D lead whose mode eigenfunction reads

$$\psi_{n,k} = \frac{1}{\sqrt{L_z}}e^{{\rm i}kz}\sqrt{\frac{2}{L_x}}\sin\frac{n\pi x}{L_x}. \tag{2.46}$$

An incoming state ψ_{n,k_n} can be scattered to another state ϕ_{m,k_m} with the same energy, and we can define the transmission amplitude $t_{m,n}(\mathcal{E})$. Therefore,

$$\psi_t^{n\to m} = t_{mn}(\mathcal{E})\sqrt{\frac{2}{L_xL_z}}\sin\frac{m\pi x}{L_x}e^{{\rm i}k_mz}, \tag{2.47}$$

and the current is

$$i^{n\to m}_{L\to R}(\mathcal{E}) = \frac{e\hbar}{mL_z}k_m(\mathcal{E})|t_{mn}(\mathcal{E})|^2. \tag{2.48}$$

Hence, for an incoming wave with energy $\mathcal{E}$ and k_n, the total transmitted current is

$$I_{L\to R}(\mathcal{E}) = \frac{e\hbar}{mL_z}\sum_m |t_{mn}(\mathcal{E})|^2k_m(\mathcal{E}). \tag{2.49}$$

The total current then reads

$$I^n_{L\to R} = \sum_{k_n>0} I_{L\to R}(\mathcal{E}(k_n))f(k_n,\mu_L) = \frac{L_z}{\pi}\int_0^\infty {\rm d}k_n\; I_{L\to R}(\mathcal{E}(k_n))f(k_n,\mu_L). \tag{2.50}$$

Since

$$\int_0^\infty {\rm d}k_n = \int {\rm d}\mathcal{E}\frac{m_e}{\hbar^2k_n(\mathcal{E})}, \tag{2.51}$$

we find

$$I^n_{L\to R} = \frac{e}{\pi\hbar}\int {\rm d}\mathcal{E}\sum_m |t_{mn}(\mathcal{E})|^2\frac{k_m(\mathcal{E})}{k_n(\mathcal{E})}. \tag{2.52}$$

Hence the total $L \to R$ current is

$$I_{L\to R} = \frac{2e}{h}\int \mathrm{d}\mathcal{E} \sum_{m,n} |t_{mn}(\mathcal{E})|^2 \frac{k_m(\mathcal{E})}{k_n(\mathcal{E})} f(\mathcal{E}, \mu_L). \tag{2.53}$$

Define

$$\tilde{t}_{mn}(\mathcal{E}) = t_{mn}(\mathcal{E})\sqrt{\frac{k_m(\mathcal{E})}{t_n(\mathcal{E})}}, \tag{2.54}$$

then

$$I_{L\to R} = \frac{2e}{h}\int \mathrm{d}\mathcal{E} \sum_{m,n} |\tilde{t}_{mn}|^2 f(\mathcal{E}, \mu_L), \tag{2.55}$$

and

$$I_{\mathrm{tot}} = \frac{2e}{h}\sum_{m,n}\int \mathrm{d}\mathcal{E}[f(\mathcal{E}, \mu_L)\tilde{T}_{mn} - f(\mathcal{E}, \mu_R)\tilde{T}'_{mn}]. \tag{2.56}$$

Current conservation demands

$$\sum_{m,n}(\tilde{T}_{mn} - \tilde{T}'_{mn}) = 0. \tag{2.57}$$

We can use the matrix form to express the total current as

$$I_{\mathrm{tot}} = \frac{2e}{h}\int \mathrm{d}\mathcal{E}\ \mathrm{tr}\Big(\mathbf{t}^\dagger\mathbf{t}\Big)[f(\mathcal{E}, \mu_L) - f(\mathcal{E}, \mu_R)]. \tag{2.58}$$

At $T = 0$, $eV \ll \varepsilon_F$, we have

$$G = \frac{2e^2}{h}\,\mathrm{tr}\Big(\mathbf{t}^\dagger\mathbf{t}\Big)|_{\varepsilon_F}. \tag{2.59}$$

2.3 Wire with Several Impurities

2.3.1 The Classical Limit

We first consider the classical limit where the quantum coherence length is way smaller than the characteristic length of the system, and suppose two impurities with transmission rates T_1 and T_2[2] are located in the lead with a distance d_0. We have shown that the total resistance should be the contact resistance R_Q pluse the intrinsic resistance introduced by the impurities, hence it suffices to choose two points A, B sandwiching the two impurities and calculate the intrinsic resistance between them.

Viewing the two impurities as a whole, it should have an effective transmission rate T_{AB} and the intrinsic resistance is

$$R_{AB} = R_Q\frac{1 - T_{AB}}{T_{AB}}, \tag{2.60}$$

[2]The missing of quantum interferences allows us to directly think about the transimission rates rather than the amplitudes.

hence we only need to calculate the transmission rate from A to B. Let's send a wave with intensity $\mathcal{A}$ from A to B, then the transmitted intensity would be

$$\mathcal{A}' = \mathcal{A}\left(T_2T_1 + T_2R_1R_2T_1 + T_2R_1^2R_2^2T_1 + \cdots\right) = \frac{T_2T_1}{1-R_2R_1}\mathcal{A}, \tag{2.61}$$

hence

$$T_{AB} = \frac{T_2T_1}{1-R_2R_1}, \tag{2.62}$$

$$R_{AB} = R_Q\frac{1-(1-T_2)(1-T_1)-T_2T_1}{T_2T_1} = R_Q\left(\frac{1-T_1}{T_1} + \frac{1-T_2}{T_2}\right). \tag{2.63}$$

Remarkably, it's exactly the addition of the intrinsic resistances of the two single impurities.

Now we can model N impurities over a length L, the average line density of the impurities is

$$\bar{n} = \frac{N}{L}. \tag{2.64}$$

Denote the average transmission rate is for each single impurity is $\bar{T}$, then the intrinsic resistance should be

$$\bar{R}_{\text{int}} = R_QN\frac{1-\bar{T}}{\bar{T}} \equiv R_Q\frac{L}{\ell_0}, \quad \ell_0 \equiv \frac{\bar{T}}{\bar{n}(1-\bar{T})}. \tag{2.65}$$

ℓ_0 is not the distance between the impurities. The total resistance is

$$R_{\text{tot}} = R_Q + R_Q\frac{L}{\ell_0} = R_Q\frac{L+\ell_0}{\ell_0}. \tag{2.66}$$

Currently this result only takes a single channel in to account. For the multichannel case where there's no inter-channel scattering and every channel share the same transmission rate, the generalized total resistance is evident

$$R_{\text{tot}} = \frac{R_Q}{M(\varepsilon_F)}\frac{L+\ell_0}{\ell_0}. \tag{2.67}$$

When $L \gg \ell_0$, an electron has to experience many impurity scatterings to be transmitted, and it is the diffusive limit where the Drude formula should be valid. In this case, our theory gives

$$R_{\text{tot}} \approx \frac{R_Q}{M(\varepsilon_F)}\frac{L}{\ell_0}, \tag{2.68}$$

while the Drude formula gives

$$R_D = \frac{1}{\sigma_D}\frac{L}{S} = \frac{m_e}{ne^2\tau}\frac{L}{S} = \frac{m_ev_F}{ne^2\ell_e}\frac{L}{S} = \frac{\hbar k_F}{n(\varepsilon_F)e^2S}\frac{L}{\ell_e}. \tag{2.69}$$

It can be shown $R_D = \alpha\frac{R_Q}{M(\varepsilon_F)}\frac{L}{\ell_e}$, where $\alpha \sim \mathcal{O}(1)$. Therefore, we can identify $\ell_0 \sim \ell_e$ as the mean free path of the scattered electron.

2.3.2 The Quantum Limit

Now let's take the phase coherence into account, then each impurity should be characterized by its transmission amplitude t_i.

We again start from the two-impurity case where the two impurities are separated by d_0 and send an incoming plane wave e^{ikz}. We have to calculated the total transmission amplitude from the left side to the right side, which is

$$t_{\text{total}} = t_2 e^{\mathrm{i}kd_0} t_1 + t_2 e^{\mathrm{i}kd_0} r_1 e^{\mathrm{i}kd_0} r_2 e^{\mathrm{i}kd_0} t_1 + \cdots = \frac{e^{\mathrm{i}kd_0} t_2 t_1}{1 - e^{2\mathrm{i}kd_0} r_2 r_1}, \tag{2.70}$$

hence

$$T_{\text{total}} = |t_{\text{total}}|^2 = \frac{T_1 T_2}{1 + R_1 R_2 - 2\,\mathrm{Re}[r_1 r_2 e^{2\mathrm{i}kd_0}]}. \tag{2.71}$$

If $t_1, t_2, r_1, r_2 \in \mathbb{R}$, then

$$T_{\text{total}} = \frac{T_1 T_2}{1 + R_1 R_2 - 2\sqrt{R_1 R_2}\cos(2kd_0)}. \tag{2.72}$$

For multi-impurity case where d_i and t_i are all random, we cannot analytically solve it. Nevertheless, we can calculate the average resistance for a two-barrier ensemble with randomized disorder distribution, hence $\phi \equiv kd_0$ randomly distributes over $[0, 2\pi]$. Since

$$R_{\text{int}} = R_Q \frac{1 - T_{\text{tot}}}{T_{\text{tot}}}, \tag{2.73}$$

we may define

$$\rho \equiv \frac{R_{\text{int}}}{R_Q} = \frac{1 - T_{\text{tot}}}{T_{\text{tot}}} = \frac{R_1 + R_2 - 2\sqrt{R_1 R_2}\cos(2\phi)}{T_1 T_2}. \tag{2.74}$$

Then the ensemble average for the disorder reads

$$\langle \rho \rangle_\phi = \frac{R_1 + R_2}{T_1 T_2} = \frac{R_1}{T_1} + \frac{R_2}{T_2} + \frac{2R_1 R_2}{T_1 T_2} \equiv \rho_1 + \rho_2 + 2\rho_1\rho_2. \tag{2.75}$$

We find $\langle \rho \rangle$ is no longer a simple addition for the two impurities, and the Ohm's law breaks down.

Now we consider a 1D wire of length L with N impurities. Again we define $\bar{n} = N/L$. The wire has an averaged $\langle \rho(L) \rangle$, and let's add a piece of $\Delta L \ll d_0$ length such that it contains at most one impurity. Then in average

$$\langle \rho(\Delta L) \rangle = \frac{R}{T} \bar{n} \Delta L, \tag{2.76}$$

and

$$\langle \rho(L + \Delta L) \rangle = \langle \rho(L) \rangle + \langle \rho(\Delta L) \rangle + 2 \langle \rho(L) \rangle \langle \rho(\Delta L) \rangle . \tag{2.77}$$

We then find

$$\frac{\partial}{\partial L}\langle\rho(L)\rangle = \frac{R\bar{n}}{T}(1+2\langle\rho(L)\rangle) = \frac{1}{\ell_0}(1+2\langle\rho(L)\rangle). \tag{2.78}$$

Since we expect $\langle\rho(0)\rangle = 0$, the solution then reads

$$\langle\rho(L)\rangle = \frac{1}{2}(e^{2L/\ell_0}-1). \tag{2.79}$$

For $L \ll \ell_0$, the leading order expansion gives

$$\langle\rho(L)\rangle \approx \frac{L}{\ell_0} \tag{2.80}$$

is the classical result. The second-order term $\Delta\rho = (L/\ell_0)^2$ gives the quantum correction. Therefore, the quantum correction to the conductance reads

$$\frac{2e^2}{h}\left(\frac{1}{\Delta\rho + L/\ell_0} - \frac{1}{L/\ell_0}\right) \approx -\frac{2e^2}{h}, \tag{2.81}$$

it's called the weak localization.

If $L \gg \ell_0$, $\langle\rho\rangle$ increases exponentially fast and the carriers are strongly localized. Now ℓ_0 is identified with the localization length ξ. In this case, the electrons' wavefunctions are localized between the impurities and diffusive motions of the charge carriers are impossible, the single-channel system falls into an insulator phase. Hopefully, in the M channel case $\xi = M\ell_0$ and diffusive motion could be possible. In this case, strong localization requires $M\ell_0 < L < \ell_\varphi$, where ℓ_φ is the quantum phase coherence length. In a cross section 200 nm × 200 nm metal, $M \sim 10^6$, $\ell \sim 1$ nm and $\xi \sim 1$ mm. However, $\ell_\varphi \ll 1$ mm, hence the strong localization is hard to be observed in 3D metals, but weak localization is feasible to observe.

2.4 Multi-terminal Devices

Now we generalize to the case where a mesoscopic device is connected to several reservoirs. Each reservoir i has chemical potential μ_i and carriers therein obey the F-D distrbution. The the total transmission rate from the reservoir j to i is characterized by T_{ij}, hence the total output of the reservoir j is

$$I_j^{\text{out}} = \frac{2e}{h}\sum_{i\neq j}\int \mathrm{d}\varepsilon\, T_{ij} f(\varepsilon,\mu_j), \tag{2.82}$$

and the total input to this reservoir is

$$I_j^{\text{in}} = \frac{2e}{h}\sum_{i\neq j}\int \mathrm{d}\varepsilon\, T_{ji} f(\varepsilon,\mu_i). \tag{2.83}$$

The net current in this reservoir then reads

$$I_j = \frac{2e}{h}\int \mathrm{d}\varepsilon\ [T_{ij}f(\varepsilon,\mu_j) - T_{ji}f(\varepsilon,\mu_i)]. \tag{2.84}$$

Current conservation then expects

$$\sum_{i\neq j}(T_{ij} - T_{ji}) = 0, \tag{2.85}$$

and

$$I_j = \frac{2e}{h}\sum_{i\neq j}\int \mathrm{d}\varepsilon\ T_{ji}[f(\varepsilon,\mu_j) - f(\varepsilon,\mu_i)]. \tag{2.86}$$

3 Classical Hall Effect

When placing a 2D electron gas in the xy-plane and imposing $\boldsymbol{B} = B\hat{e}_z$ and apply $\boldsymbol{E} = E\hat{e}_x$, a Hall voltage can be measured along the y-direction.

It's calssically expalined by the Lorentz force $\boldsymbol{F}_L = q\boldsymbol{v}\times\boldsymbol{B} = \boldsymbol{j}_x\times\boldsymbol{B}/n_s = -\frac{1}{n_s}j_xB\hat{e}_y$ makes the electrons accumulate at one edge of the wire to create a repulsive force $\boldsymbol{F}_e$ balancing $\boldsymbol{F}_L$ such that in the steady state $\boldsymbol{F}_e + \boldsymbol{F}_L = 0$. This creates a y-direction electric field

$$\boldsymbol{E}_H = \frac{\boldsymbol{F}_e}{q} = \frac{j_xB}{n_sq}\hat{e}_y, \tag{3.1}$$

hence the Hall voltage reads $V_H = j_xd_yB/qn_s = I_xB/n_sq$, and the Hall resistivity is defined as $\rho_H = V_H/j_x = \frac{B}{n_sq}$.

A more detailed analysis can base on the Drude model. At the stationary state we have

$$m\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = q(\boldsymbol{E} + \boldsymbol{v}\times\boldsymbol{B}) - \frac{m}{\tau}\boldsymbol{v} = 0, \tag{3.2}$$

$$q\begin{pmatrix}E_x + v_yB\\ E_y - v_xB\end{pmatrix} - \frac{m}{\tau}\begin{pmatrix}v_x\\ v_y\end{pmatrix} = 0. \tag{3.3}$$

Hence

$$\begin{pmatrix}E_x\\ E_y\end{pmatrix} = \begin{pmatrix}\frac{m}{q\tau} & -B\\ B & \frac{m}{q\tau}\end{pmatrix}\begin{pmatrix}v_x\\ v_y\end{pmatrix} = \begin{pmatrix}\frac{m}{n_s\tau q^2} & -\frac{B}{n_sq}\\ \frac{B}{n_sq} & \frac{m}{n_s\tau q^2}\end{pmatrix}\begin{pmatrix}j_x\\ j_y\end{pmatrix}. \tag{3.4}$$

We usually define $\sigma_0 = \frac{\tau}{m}n_sq^2 \equiv \mu n_sq^2$, where $\mu = \tau/m$ is called the mobility. The Hall effect corresponds to $j_y = 0$, and the resistivity reads

$$\rho_H = \frac{E_y}{j_x} = \frac{B}{n_sq}. \tag{3.5}$$

Agree with the crude analysis before, and it's sensitive to the carrier's charge and the carrier's density.

4 Electrons in the Magnetic Field and The IQHE

According to the minimal substitution, the single-electron Hamiltonian coupled to the magnetic field reads

$$H = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A})^2 + q\phi, \tag{4.1}$$

and the gauge invariance $\boldsymbol{A} \to \boldsymbol{A} + \nabla\chi$, $\phi \to \phi - \partial_t\chi$ demands the wavefunction transforms as

$$\psi \to e^{\mathrm{i}\frac{q}{\hbar}\chi}\psi. \tag{4.2}$$

The current density reads

$$\boldsymbol{j} = q\,\mathrm{Re}\,\langle\psi|\hat{\boldsymbol{p}} - q\hat{\boldsymbol{A}}|\psi\rangle\,. \tag{4.3}$$

Foe 2D electron gas under the perpendicular magnetic field $\boldsymbol{B} = B\hat{e}_z$, the vector potential can be chose as

$$\boldsymbol{A} = (0, xB, 0), \tag{4.4}$$

and the Hamiltonian reads

$$H = \frac{1}{2m}[p_x^2 + (p_y - qBx)^2]. \tag{4.5}$$

The y-translation sym is preserved, the eigenfunction can be written as

$$\psi(x, y) = u_{k_y}(x)e^{\mathrm{i}k_y y}, \tag{4.6}$$

and

$$\frac{1}{2m}(p_y - qBx)^2\psi = \frac{1}{2m}(\hbar k_y - qBx)^2\psi = \frac{(qB)^2}{2m}(x - k_y\ell_B^2)^2\psi, \tag{4.7}$$

where we define the magnetic length ℓ_B as

$$\ell_B \equiv \sqrt{\frac{\hbar}{eB}}. \tag{4.8}$$

Therefore,

$$\frac{1}{2m}[p_x^2 + (eB)^2(x - k_y\ell_B^2)^2]u_{k_y}(x) = Eu_{k_y}(x). \tag{4.9}$$

Denote

$$x_{k_y} = k_y\ell_B^2, \qquad \omega_c = \frac{eB}{m}, \tag{4.10}$$

we find

$$\left[\frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2(x - x_{k_y})^2\right]u_{k_y}(x) = Eu_{k_y}(x), \tag{4.11}$$

which is exactly an harmonic oscillator centered at x_{k_y}. Therefore, the energy spectrum of this electron is discretized into Landau levels

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right), \tag{4.12}$$

and an eigenstate is labelled as ψ_{n,k_y}. $|\psi_{n,k_y}|^2$ is localized at x_{k_y} with a variance characterized by ℓ_B.

Suppose the sample's size along y is L_y, then $\delta k_y = \frac{2\pi}{L_y}$ and $\delta x_k = \frac{2\pi\ell_B^2}{L_y}$. Hence, the degeneracy of each Landau level is characterized by

$$g = \frac{L_x}{\delta x_k} = \frac{L_x L_y eB}{2\pi\hbar} = \frac{SBe}{h} = \frac{\Phi}{\phi_0}, \tag{4.13}$$

where we define the flux quantum $\phi_0 = h/e$. We define n_L as the available state per unit of surface,

$$n_L = \frac{g}{S} = \frac{eB}{h}, \tag{4.14}$$

and n_s is the carrier's density at the Landau level's energy, we then define the filling factor as

$$\nu = \frac{n_s}{n_L} = \frac{hn_s}{eB}. \tag{4.15}$$

Suppose the external voltage is imposed along the y direction and the width along the x direction is denoted as W. Then the edges introduce confining potentials at the boundary $V(x)$. It pushes up the energy of the state (n, k_y) near the edge to

$$\mathcal{E}(n, x_k = k_y\ell_B^2) = \hbar\omega_c\left(n + \frac{1}{2}\right) + V(k_y\ell_B^2), \tag{4.16}$$

which could approach the Fermi energy, making the group velocity reads

$$v_y = \frac{1}{\hbar}\frac{\partial\mathcal{E}}{\partial k_y} = \frac{1}{eB}\left.\frac{\partial V(x)}{\partial x}\right|_{x=k_y\ell_B^2}. \tag{4.17}$$

Since $V(x)$ has opposite slopes at the opposite edges, and is flat in the center of the strip, we find the carriers are moving in the opposite directions along the opposite edges, and is static in the center. When there is no external voltage bias, the net current transported by the edge states is zero.

Now suppose one reservoir connecting to the sample along the y direction has μ_1, another has μ_2. The net current reads

$$I = I_{1\to 2} - I_{2\to 1}. \tag{4.18}$$

In the Landauer formalism,

$$I_{1\to 2} = \frac{q}{L_y}\sum_{k>0}\frac{\hbar k_y}{m}f(k, \mu_1) = \frac{eg}{h}\int \mathrm{d}\varepsilon\ f(\varepsilon, \mu_1), \tag{4.19}$$

g denotes the degeneracy of (n, k_y) due to spin or other reasons. The net current then reads

$$I = \frac{ge^2}{h}V. \tag{4.20}$$

If m Landau levels are filled, it naturally generalizes to

$$I_m = \frac{mge^2}{h}V. \tag{4.21}$$

Each Landau level is perfectly transmitted (ballistic), and the current is localized on the edge. Even if scatter occurs between two Landau levels with the same energy, the carrier still goes to the same direction, i.e., no backscatterings.

5 Superconductivity

Superconductivity is the most common macroscopic quantum coherent phenomenon. A superconducting phase is of an infinite conductance, and it has the Meissner effect, i.e., it is a perfect diamagnet up to a critical field B_c, meaning applying $\boldsymbol{B}$ creates a screening current at the surface of the superconductor such that the magnetic field is zero in the bulk. Type-I superconductor loses the superconductivity for $B > B_c$, while the Type-II superconductor gradually loses the Meissner effect for $B_{c1} < B < B_{c2}$ (the magnetic field penetrates the material creating vortices) and loses the superconductivity for $B > B_{c2}$.

The critical magnetic field $H_c(T)$ behaves a temperature dependence

$$H_c(T) = H_c(0)\left(1 - \frac{T}{T_c}\right)^2, \tag{5.1}$$

and it can be derived from the Ginzburg-Landau theory later. In particular, the Gibbs free-energy $G(T, H)$ abruptly changes upon a normal-superconducting phase transition:

$$G_{\text{normal}}(T, 0) - G_{\text{superconductor}}(T, G) = \Delta G(T) = \frac{1}{2}\mu_0 H_c^2(T), \tag{5.2}$$

therefore the critical magnetic field $H_c(T)$ breaks the superconducting phase basically by lifting the free energy to the normal phase. The zero-field normal-superconductor phase transition at T_c is a second-ordr transition, while the superconductor-normal transition at $T < T_c$ induced by $H > H_c(T)$ is a first-order one with a finite latent heat.

5.1 Phenomenological Explanation

The characters of superconductivity can be well reproduced by describing the electrons near the Fermi surface in a superconductor by a single macroscopic wavefunction

$$\psi(\boldsymbol{r}) \equiv \sqrt{n(\boldsymbol{r})}e^{\mathrm{i}\Theta(\boldsymbol{r})}, \tag{5.3}$$

where $n(\boldsymbol{r})$ is the density of carriers (Cooper pairs) in a superconductor, and $\Theta(\boldsymbol{r})$ is the collective phase for all carriers. Therefore,

$$\int |\psi|^2 \mathrm{d}\boldsymbol{r} = \int n(\boldsymbol{r})\mathrm{d}\boldsymbol{r} \equiv N_s \tag{5.4}$$

describes the total number of condensated Cooper pairs. As we have mentioned, when coupled to a magnetic field, the current density reads

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{q}{m}\,\mathrm{Re}[\psi^*(\boldsymbol{r})(-\mathrm{i}\hbar\nabla - q\boldsymbol{A})\psi(\boldsymbol{r})]. \tag{5.5}$$

It's natural to assume $n(\boldsymbol{r}) = n_s$ is independent of $\boldsymbol{r}$, hence

$$\boldsymbol{j}_s(\boldsymbol{r}) = \frac{\hbar q n_s}{m}\left(\nabla\Theta(\boldsymbol{r}) - \frac{q}{\hbar}\boldsymbol{A}\right) \tag{5.6}$$

Note two electons compromise a Cooper pair, hence $q = 2e$, $m = 2m_e$.

Now we find

$$\nabla\times\boldsymbol{j}_s = -\frac{q^2 n_s}{m}\nabla\times\boldsymbol{A} = -\frac{q^2 n_s}{m}\boldsymbol{B}. \tag{5.7}$$

Since $\nabla\times\boldsymbol{B} = \mu_0\boldsymbol{j} + \mu_0\varepsilon_0\partial_t\boldsymbol{E}$, in the absence of varying electric field we find

$$\begin{aligned}\nabla\times(\nabla\times B) &= \varepsilon_{ijk}\varepsilon_{k\ell m}\partial_j\partial_\ell B_m\hat{e}_i = (\delta_{i\ell}\delta_{jm} - \delta_{im}\delta_{j\ell})\partial_j\partial_\ell B_m\hat{e}_i = -\nabla^2\boldsymbol{B}\\ &= \mu_0\nabla\times\boldsymbol{j} = -\frac{\mu_0 n_s q^2}{m}\boldsymbol{B},\end{aligned} \tag{5.8}$$

i.e.

$$\nabla^2 B - \frac{\mu_0 n_s q^2}{m}\boldsymbol{B} \equiv \nabla^2\boldsymbol{B} - \frac{1}{\lambda_L^2}\boldsymbol{B} = 0, \tag{5.9}$$

where we defined $\lambda_L^2 \equiv \frac{m}{\mu_0 n_s q^2} \sim 10$ nm as the Lodon penetration length, and this equation is the second London equation describing an exponentially supressed external magnetic field in a superconductor.

Since $\nabla\times\boldsymbol{E} = -\partial_t\boldsymbol{B}$, we find

$$\nabla\times(\partial_t\boldsymbol{j}) = -\frac{n_s q^2}{m}\partial_t\boldsymbol{B} = \frac{n_s q^2}{m}\nabla\times\boldsymbol{E}, \tag{5.10}$$

hence

$$\partial_t\boldsymbol{j} = \frac{n_s q^2}{m}\boldsymbol{E} = \frac{1}{\mu_0\lambda_L^2}\boldsymbol{E}. \tag{5.11}$$

This is the first London equation demonstrating the prefect conductivity:superconductor: If $\boldsymbol{j}$ is constant, then $\boldsymbol{E} = 0$ implies $\boldsymbol{E} = 0$, hence infinite σ; whereas if $\boldsymbol{E} = \boldsymbol{E_0}e^{\mathrm{i}\omega t}$, then

$$\boldsymbol{j}_s(t) = \frac{1}{\mathrm{i}\mu_0\omega\lambda_L^2}\boldsymbol{E_0}e^{\mathrm{i}\omega t} \;\Rightarrow\; \sigma = \frac{1}{\mathrm{i}\mu_0\omega_0\lambda_L^2}, \tag{5.12}$$

we have a pure imaginary conductivity, implying there's no dissipation and the superconductor is a pure inductance.

The simple phenomenological model also captures the flux quantization, saying the flux penetrating a superconductor ring is quantized. Notice that the screening current only flows on the surface of the SC, but inside of the SC we have $\boldsymbol{j} = 0$. Let's consider a

closed path $\mathscr{C}$ along the ring in the superconductor, we find

$$\boldsymbol{j}_s(\boldsymbol{r}) = \frac{\hbar q n_s}{m}\left(\nabla\Theta(\boldsymbol{r}) - \frac{q}{\hbar}\boldsymbol{A}\right) = 0, \tag{5.13}$$

hence

$$\nabla\Theta(\boldsymbol{r}) = \frac{q}{\hbar}\boldsymbol{A}. \tag{5.14}$$

Hence

$$\oint_{\mathscr{C}} \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{l} = \frac{\hbar}{q}\oint_{\mathscr{C}} \nabla\Theta\cdot \mathrm{d}\boldsymbol{l}, \tag{5.15}$$

hence

$$\Phi = \frac{\hbar}{q}2\pi n = n\phi_0, \tag{5.16}$$

where $\phi_0 = h/q$ is the flux quantum. This flux quantization serves as a concrete manifestation of a quantum mesoscopic effect. We again stress here $q = 2e$.

5.2 The Landau Theory

According to Landau's idea, we can expand the gauge-invariant reduced free energy in powers of $|\psi|$ and find

$$f(T,\psi) = f_0(T) + a(T)|\psi|^2 + \frac{b_0}{2}|\psi|^4, \tag{5.17}$$

the linear and the third order terms vanish as they are not gauge-invariant. The extrema of this free energy are

$$|\psi| = 0,\ \sqrt{-\frac{a}{b}}. \tag{5.18}$$

If $|\psi| = 0$ is the minimum, then there's no finite Cooper pair density, hence corresponds of the normal phase; whereas $|\psi| = \sqrt{-\frac{a}{b}}$ does gives Cooper pair condensation and brings the superconductivity. Whether an extremum is the a minimum is inspected through the second order derivative:

$$\frac{\partial^2 f}{\partial\psi^2} = 2a + 6b|\psi|^2 \overset{?}{>} 0, \tag{5.19}$$

hence for $a > 0$, $|\psi| = 0$ is the only minimum; while if $a < 0$, the minimum condition reads

$$|\psi_s| = \sqrt{n_s} > \sqrt{-\frac{a}{3b}}, \tag{5.20}$$

which is satisfied by $|\psi| = \sqrt{-\frac{a}{b}}$.

Now we see the critical temperature T_c corresponds to $a(T_c) = 0$, and there should be $a(T > T_c) > 0$ and $a(T < T_c) < 0$. (We assume b_0 is constant.) $a(T)$ can be linearized to

$$a(T) = a_0(T - T_c) \tag{5.21}$$

in the neighborhood of T_c, and we finally find

$$|\psi_s|^2 = n_s = \frac{a_0}{b_0}(T_c - T). \tag{5.22}$$

This relation is experimentally verified around T_c.

$f_0(T)$ then can be interpreted as the free energy of the normal phase, hence the energy difference between the normal phase adn the superconducting phase is given by

$$\Delta f = a_0(T - T_c)|\psi_s|^2 + \frac{b_0}{2}|\psi_s|^4 = -\frac{a_0^2}{b_0}(T - T_c)^2 + \frac{a_0^2}{2b_0}(T - T_c)^2 = -\frac{a_0^2}{2b_0}(T_c - T)^2. \tag{5.23}$$

Therefore, for $T < T_c$, the superconducting phase is indeed of a lower energy.

To study the effect of magnetic field, we can couple $\boldsymbol{B}$ to the free energy by adding the term

$$\Delta f_B^{(\mathrm{SC})} = -\int_0^B m\mathrm{d}B = \int_0^B \frac{B}{\mu_0}\mathrm{d}B = \frac{B^2}{2\mu_0} = \frac{1}{2}\mu_0 H^2, \tag{5.24}$$

to the superconducting phase, note in a SC $m = -H = -B/\mu_0$. While for the normal phase, we have

$$\Delta f_B^{(\mathrm{nor})} = -\frac{1}{\mu_0}\int_0^B \chi B\mathrm{d}B \sim 0, \tag{5.25}$$

hence an applied magnetic field lifts the energy of the superconducting phase. Clearly, the superconductivity is ruined when

$$\frac{1}{2}\mu_0 H^2 = |\Delta f| = \frac{a_0^2}{2b_0}(T_c - T)^2, \tag{5.26}$$

giving a critical magnetic field

$$H = \frac{a_0}{\sqrt{b_0\mu_0}}(T_c - T). \tag{5.27}$$

We can also calculate the thermodynamic observables using the pheno free energy. The reduced entropy reads

$$s = -\frac{\partial f}{\partial T} = -\frac{\partial f_0}{\partial T} + \frac{a_0^2}{b_0}(T - T_c), \tag{5.28}$$

for $T < T_c$, while it equals to $-\partial f_0/\partial T$ for $T > T_c$. The entropy is continuous at T_c, thus it is a continuous phase transition. However, the heat capacity gives

$$c = T\frac{\partial S}{\partial T} = \begin{cases} -T\dfrac{\partial^2 f_0}{\partial T^2}, & T > T_c, \\ -T\dfrac{\partial^2 f_0}{\partial T^2} + T\dfrac{a_0^2}{b_0}, & T < T_c. \end{cases} \tag{5.29}$$

It's discontinuous at T_c. Therefore, the superconductivity transition is a second-order phase transition.

5.3 The Ginzburg-Landau Theory

Now let's allow $n_s(\boldsymbol{r})$ to be inhomogeneous. In this case, the Ginzburg-Landau free energy acquires a kinetic term and reads

$$F_{\mathrm{GL}} = F_0 + \int \mathrm{d}\boldsymbol{r}\ \frac{\hbar^2}{2m}|\nabla\psi|^2 + a(T)|\psi(\boldsymbol{r})|^2 + \frac{b_0}{2}|\psi(\boldsymbol{r})|^4. \tag{5.30}$$

Now we find the EoM of $\psi(\boldsymbol{r})$ reads

$$-\frac{\hbar^2}{2m}\nabla^2\psi + [a(T) + b_0|\psi(\boldsymbol{r})|^2]\psi(\boldsymbol{r}) = 0. \tag{5.31}$$

It's generally hard to solve. Nevertheless, we can study the 1D case at the interface of a superconductor and a normal phase (here we take it to be vacuum for $x < 0$). $\psi(x)$ in the superconductor satisfies

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + [a(T) + b_0|\psi|^2]\psi = 0. \tag{5.32}$$

Under the boundary consition $\psi(x < 0) = 0$, the solution is

$$\psi(x) = \psi_0\frac{x}{\xi\sqrt{2}}, \quad \xi \equiv \frac{\hbar^2}{2m|a(T)|}, \quad \psi_0 = \sqrt{-\frac{a}{b}}. \tag{5.33}$$

ξ is named the superconducting coherence length. It's worth noting that $\lim_{T\to T_c-0}\xi(T) \to \infty$, agree with the picture that ξ diverges at the transition point.

Now we can couple the Ginzburg-Landau functional to a magnetic field. Since $\boldsymbol{p} - q\boldsymbol{A} = \boldsymbol{p} + 2e\boldsymbol{A}$, we find

$$f = f_0 + a(T)|\psi(\boldsymbol{r})|^2 + \frac{b_0}{2}|\psi(\boldsymbol{r})|^4 + \frac{1}{2m}|(-\mathrm{i}\hbar\nabla + 2e\boldsymbol{A})\psi(\boldsymbol{r})|^2 + \frac{1}{2\mu_0}(\nabla\times\boldsymbol{A})^2. \tag{5.34}$$

Minimize this functional with respect to $\boldsymbol{A}$ gives

$$\boldsymbol{j}_s = \frac{\mathrm{i}\hbar e}{m}(\psi\nabla\psi^* - \psi^*\nabla\psi) + \frac{(2e)^2}{m}|\psi|^2\boldsymbol{A} = \frac{1}{\mu_0}\nabla\times\boldsymbol{B}. \tag{5.35}$$

Substituting $\psi(\boldsymbol{r}) = \sqrt{n_s(\boldsymbol{r})}e^{\mathrm{i}\Theta(\boldsymbol{r})}$ gives

$$\boldsymbol{j}_s = \frac{2\hbar e}{m}|\psi|^2\left(\nabla\Theta + \frac{2e}{\hbar}\boldsymbol{A}\right). \tag{5.36}$$

The result of the previous pheno approach is recovered, and it reproduces another characteriztic length λ describing the deacy of $\boldsymbol{B}$ in a superconductor (the Meissner effect).

The ratio $\kappa \equiv \lambda(T)/\xi(T)$ is the Ginzburg-Landau parameter classifying the type of the superconductor. $\kappa < 1$ gives the type-I superconductor, while $\kappa > 1$ corresponds to the type-II one. When placed in a magnetic field, the free energy of a pure superconductor's

interface is estimated to be

$$f_s \sim f_S(H)\lambda^2, \tag{5.37}$$

while if a vortex with core size ξ is formed on the surface, the free energy is esitmated to be

$$f_v \sim f_S(0)(\lambda^2 - \xi^2) + f_N(0)\xi^2. \tag{5.38}$$

Note $\frac{1}{2}\mu_0 H_c^2 = f_N(0) - f_s(0)$ and $f_s(H) = f_s(0) + \frac{1}{2}\mu_0 H^2$, we find

$$f_s - f_v = \frac{1}{2}\mu_0 H^2\lambda^2 - \frac{1}{2}\mu_0 H_c^2\xi^2. \tag{5.39}$$

A vortex is favored when $f_s - f_v > 0$, hence

$$H > H_c\frac{\xi}{\lambda}. \tag{5.40}$$

However, H should be less that H_c to preserve the residual SC phase, hence a vortex forming demands $\kappa > 1$, and $H_{c1} = H_c\frac{\xi}{\lambda} < H_c$.

For a type-II superconductor, the second critical field corresponds to the case where there are too many vortices that the SC regions are disconnected. A crude estimation is a $S \sim \pi\xi^2$ vortex has a flux quantum ϕ_0, and the maximal number of vortices an area S can hold is

$$N = \frac{S}{\pi\xi^2}. \tag{5.41}$$

Hence

$$B_{c2} = \frac{N\phi_0}{S} = \frac{\phi_0}{\pi\xi^2}. \tag{5.42}$$

Meanwhile, the pheno model gives

$$B_{c1} = \mu_0 H_{c_1} = \frac{\phi_0}{\pi\lambda^2}. \tag{5.43}$$

Clearly, for $B_{c1} < B_{c2}$ we again requires $\kappa > 1$.

5.4 Vortices

We can analytically study the vortex configuration.

$$\boldsymbol{j}_s = \frac{2\hbar e}{m}|\psi|^2\left(\nabla\Theta + \frac{2e}{\hbar}\boldsymbol{A}\right) \tag{5.44}$$

gives

$$\boldsymbol{A} = \frac{m}{(2e)^2|\psi|^2}\boldsymbol{j}_s + \frac{\hbar}{2e}\nabla\Theta. \tag{5.45}$$

Take any closed path $\mathscr{C}$ in SC and integrate over it gives

$$\Phi = \frac{m}{2e}\oint_{\mathscr{C}} \mathrm{d}\boldsymbol{l}\cdot\boldsymbol{v}_s + \frac{\hbar}{2e}\oint_{\mathscr{C}} \mathrm{d}\boldsymbol{l}\cdot\nabla\Theta = \frac{m_e}{e}\oint_{\mathscr{C}} \mathrm{d}\boldsymbol{\ell}\cdot\boldsymbol{v}_s \pm \frac{nh}{2e}. \tag{5.46}$$

Note $\boldsymbol{j}_s = n_s q \boldsymbol{v}_s = 2e n_s \boldsymbol{v}_s$. Thefore, the flux in a vortex can only vary an integer times of the flux quantum. In realistic materials, the vortices are pinned by impurities, and as $B \to B_{c2}^-$, the vortices will arrange in a periodic structure called the Abrikosov lattice.

Now let's look for a vortex solution with the boundary condition

$$\psi(0) = 0, \quad \psi(r \to \infty) = \psi_0, \quad B(r \to \infty) = 0, \tag{5.47}$$

under the ansatz

$$\psi(\boldsymbol{r}) = |\psi(r)| e^{\mathrm{i}\Theta}, \quad \boldsymbol{v}_s(\boldsymbol{r}) = v_s(r)\hat{e}_\phi, \quad \boldsymbol{B}(\boldsymbol{r}) = B(r)\hat{e}_z. \tag{5.48}$$

Therefore,

$$\boldsymbol{A}(\boldsymbol{r}) = A(r)\hat{e}_\phi, \quad B(\boldsymbol{r}) = \frac{1}{r}\frac{\partial}{\partial r}[rA(r)] \tag{5.49}$$

For $R \gg \xi$, we expect

$$\phi_0 = \Phi(R) - \frac{m_e}{e}\oint \mathrm{d}\boldsymbol{\ell} \cdot \boldsymbol{v}_s = 2\pi R\left[A(R) - \frac{v_s m_e}{e}\right], \tag{5.50}$$

hence

$$A(r) = \frac{\phi_0}{2\pi R} + \frac{m_e v_s}{e}. \tag{5.51}$$

For $r, \lambda \gg \xi$, then magnetic field satisfies

$$B - \nabla^2 B = \phi_0 \delta^2(\boldsymbol{r}), \tag{5.52}$$

the solution is written in the Bessel function

$$\boldsymbol{B}(r) = \frac{\phi_0}{2\pi\lambda^2} K_0\left(\frac{r}{\lambda}\right)\hat{e}_z. \tag{5.53}$$

Suppose the vortex tube is of length L, the energy of the vortex outskirt is computed as

$$F_{v,o} = L\int \mathrm{d}^2\boldsymbol{r}\left[\frac{\boldsymbol{B}^2}{2\mu_0} + \frac{\lambda^2}{2\mu_0}(\nabla \times \boldsymbol{B})^2\right] \approx L\frac{\phi_0^2}{2\pi\lambda^2}\ln\frac{\lambda}{\xi} + \cdots, \tag{5.54}$$

while the core energy is estimated to be $F_{\mathrm{cor}} = \pi\xi^2 \frac{B_c^2}{2\mu_0}$. Moreover, interaction between two vortices scales as $K_0(|r_1 - r_2|/\lambda)$, hence is asymptotically log-interaction.