

Temperature and thermometry

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I. TEMPERATURE IN STATISTICAL PHYSICS

Consider two systems 1 and 2 coupled to each other, see Fig.1. let E_1 and E_2 be the energies of them, such that $E = E_1 + E_2 = \text{constant}$, i.e. the combined system is isolated from the rest of the world. The corresponding number of available microstates in each subsystem is $\Omega_1(E_1)$ and $\Omega_2(E_2)$, respectively. The whole system can be in any of the $\Omega_1(E_1)\Omega_2(E_2)$ available microstates. We assume that the two bodies have been in contact long enough such that they have reached equilibrium. The idea is that the combined system will choose a macroscopic configuration that maximizes the number of the microstates.

Assumptions:

(1) each one of the possible microstates of a system is equally likely to occur;

(2) given enough time, the system will explore all possible microstates and spend equal time in each of them.

Next, we maximize $\Omega_1(E_1)\Omega_2(E_2)$ with respect to $E_1 = E - E_2$

$$\frac{d}{dE_1}(\Omega_1(E_1)\Omega_2(E_2)) = 0 \quad (1)$$

$$\Omega_2(E_2)\frac{d\Omega_1(E_1)}{dE_1} + \Omega_1(E_1)\frac{d\Omega_2(E_2)}{dE_2}\frac{dE_2}{dE_1} = 0. \quad (2)$$

Since $dE_1 = -dE_2$, Eq. (1) becomes

$$\frac{d \ln \Omega_1}{dE_1} = \frac{d \ln \Omega_2}{dE_2}. \quad (3)$$

We define the temperature T by

$$\frac{1}{k_B T} = \frac{d \ln \Omega}{dE}, \quad (4)$$

where $k_B = 1.3806 \times 10^{-23} \text{ JK}^{-1}$ is the Boltzmann constant, therfor $T_1 = T_2$. Equation (4) is consistent with entropy in statistical mechanics $S = k_B \ln \Omega$ and $dE = TdS$.

II. ENSEMBLES

There are three main ensembles used in thermal physics:

(1) **The microcanonical ensemble:** a statistical ensemble that represents the possible states of a system with specified energy.

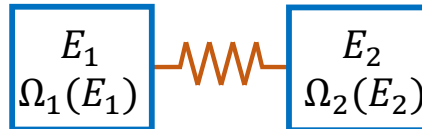


FIG. 1: Two systems are exchanging energy with each other.

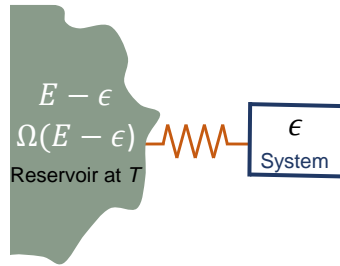


FIG. 2: A reservoir (heat bath) at temperature T connected to a system.

(2) The canonical ensemble: represents the possible states of a system that can exchange its energy with a large reservoir. This fixes (and defines) the temperature of the system.

(3) The grand canonical ensemble: represents the possible states of a system which can exchange both energy and particles with a large reservoir. This fixes the systems temperature and the systems chemical potential μ .

III. CANONICAL ENSEMBLE

We consider a system exchanging energy with a reservoir (heat bath) as shown in Fig. 2. Heat bath is such a big reservoir that its properties do not change, in particular temperature, by taking or adding energy to/from it. We assume that for each allowed energy of the system there is only a single microstate, and therefore the system has a value $\Omega = 1$. We fix the total energy of the system plus reservoir to be E . The energy of the reservoir is taken to be $E - \epsilon$ while the energy of the system is taken to be ϵ . This situation of a system in thermal contact with a large reservoir is the canonical ensemble as shown in the Fig.2.

The probability $p(\epsilon)$ that the system has energy ϵ is proportional to the number of microstates which are accessible to the reservoir multiplied by the number of microstates which are accessible to the system. Therefore

$$p(\epsilon) \propto \Omega(E - \epsilon) \times 1 \quad (5)$$

Since temperature has a logarithmic dependence of Ω , and since $\epsilon \ll E$, we can perform Taylor expansion of $\ln(E - \epsilon)$ around $\epsilon = 0$ up to the first order, so that

$$\ln \Omega(E - \epsilon) = \ln \Omega(E) - \frac{d \ln \Omega(E)}{dE} \epsilon. \quad (6)$$

Then we have

$$\Omega(E - \epsilon) = \Omega(E) e^{-\epsilon/k_B T}, \quad (7)$$

where T is the temperature of the reservoir. Using Eq. (5), the probability distribution describing the system is thus given by

$$p(\epsilon) \propto e^{-\epsilon/k_B T}. \quad (8)$$

The system is now in equilibrium with the reservoir. However, its energy ϵ is not a constant but is governed by the probability distribution in Eq. (8). This is known as the Boltzmann distribution and also as the canonical distribution. The term $e^{-\epsilon/k_B T}$ is known as a Boltzmann factor. To quantify this distribution properly we need to normalize it. If a system is in contact with a reservoir and has a microstate i with energy E_i , then

$$p(\text{microstate } i) = \frac{e^{-E_i/k_B T}}{\sum_j e^{-E_j/k_B T}}, \quad (9)$$

where $Z \equiv \sum_j e^{-E_j/k_B T}$ is the partition function.

IV. EXAMPLE: TWO LEVEL SYSTEM (TLS)

As the simplest application of the canonical ensembles, we consider a two-state system with energies $E_g = 0$ and $E_e = \epsilon$. Here the subscript g and e refer to ground and excited state, respectively. This system is in thermal contact to a heat bath at temperature T . In accordance with Eq. (9), the probabilities that the TLS is either in the ground or excited state, p_g and p_e , are given by

$$\begin{aligned} p_g &= \frac{1}{1 + e^{-\epsilon/k_B T}} \\ p_e &= 1 - p_g = \frac{e^{-\epsilon/k_B T}}{1 + e^{-\epsilon/k_B T}}. \end{aligned} \quad (10)$$

The expectation value of the energy is then

$$\langle E \rangle = 0 \times p_g + \epsilon p_e = \frac{\epsilon}{1 + e^{\epsilon/k_B T}}. \quad (11)$$

V. SHORTCUTS TO FERMI-DIRAC AND BOSE-EINSTEIN DISTRIBUTION

A. Fermi-Dirac distribution

Assume the single-particle state ϵ is a grand canonical ensemble. For this the partition function based on Pauli exclusion principle reads

$$\begin{aligned} Z &= e^{-\beta \times 0} + e^{-\beta(\epsilon - \mu)} \\ &= 1 + e^{-\beta(\epsilon - \mu)}, \end{aligned} \quad (12)$$

where $\beta \equiv 1/(k_B T)$ and μ is the chemical potential of the system. The partition function here is $Z = e^{-\beta \Phi}$, where Φ is called the grand potential of the system. In general, the grand potential of a system is given by

$$\Phi = \langle E \rangle - TS - \mu \langle N \rangle, \quad (13)$$

where $\langle N \rangle$ is the average occupation in the state ϵ ,

$$\langle N \rangle = -\frac{\partial \Phi}{\partial \mu} = \frac{1}{\beta Z} \frac{dZ}{d\mu} = \frac{1}{1 + e^{\beta(\epsilon - \mu)}}. \quad (14)$$

Here we identify the population $\langle N \rangle$ with the distribution

$$f(\epsilon) = \frac{1}{1 + e^{\beta(\epsilon - \mu)}} \quad (15)$$

i.e. the Fermi-Dirac distribution function.

B. Bose-Einstein distribution

With the same procedure as in the previous subsection, we again consider a single-particle state as a grand canonical system. Unlike the previous case, here for bosons multiple occupations are allowed whereby the partition function reads

$$Z = \sum_{N=0}^{\infty} e^{-N\beta(\epsilon - \mu)} = \frac{1}{1 - e^{-\beta(\epsilon - \mu)}}, \quad (16)$$

where we summed the geometric series in the second step. Then as before we find the average occupation $\langle N \rangle = \frac{1}{\beta Z} \frac{dZ}{d\mu} = \frac{1}{e^{\beta(\epsilon - \mu)} - 1}$, and we again identify the population $\langle N \rangle$ with the distribution

$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu)} - 1} \quad (17)$$

i.e. the Bose-Einstein distribution function.

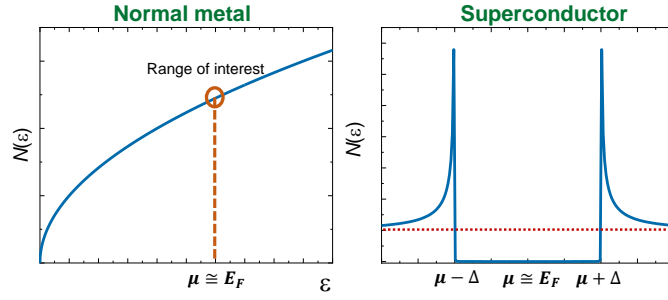


FIG. 3: DOS (a) for normal metal over wide energy range and (b) for superconductor around the Fermi level. Note: In (b) the dashed line corresponds to DOS in the normal state.

VI. DENSITY OF STATES

Before discussing thermometry in electronic systems, we need some further prerequisites. We deal with a 3D electron gas, since the Fermi wavelength $\lambda_F \ll d$, where d is the smallest dimension of the sample we consider. Typically $\lambda_F < 1$ nm for a metal and dimensions of structures to be presented are $d \sim 100$ nm or larger. In this case the density of states (DOS) is proportional to $\sqrt{\epsilon}$. The Fermi temperature $E_F/k_B \sim 10^5$ K for typical metals. This means that both the operating temperature of $T \leq 1$ K, and similarly bias voltages $V \sim 1$ mV with $eV/k_B \sim 10$ K are in the range of $\ll E_F/k_B$. Therefore we can safely approximate the density of states in the normal state as constant $N(E_F)$ over these relevant energies around the Fermi level (see Fig. 3a). For ordinary superconductors we have BCS DOS $N(\epsilon) = n_S(\epsilon)N(E_F)$ where $n_S(\epsilon) = |\epsilon|/\sqrt{\Delta^2 - \epsilon^2}$ for $|\epsilon| > \Delta$ and $n_S(\epsilon) = 0$ otherwise. Here Δ is the energy gap of the superconductor (Fig. 3b). As an example $\Delta/k_B \sim 2$ K for Al.

VII. PHENOMENOLOGICAL DERIVATION OF TUNNELING CURRENT

Consider two conductors which are separated by an insulator. This forms the tunnel junction as shown in Fig. 4a. Quantum mechanically, electrons can tunnel through a potential barrier formed by the insulating layer from one electrode to the other, resulting in current flow through the junction. The forward and backward tunneling rates, Γ_f and Γ_b , are given by

$$\begin{aligned}\Gamma_f &= |\mathcal{T}|^2 \int d\epsilon n_L(\epsilon) f_L(\epsilon) n_R(\epsilon + eV) [1 - f_R(\epsilon + eV)] \\ \Gamma_b &= |\mathcal{T}|^2 \int d\epsilon n_R(\epsilon + eV) f_R(\epsilon + eV) n_L(\epsilon) [1 - f_L(\epsilon)],\end{aligned}\quad (18)$$

where $|\mathcal{T}|^2$ is the "transparency" of the junction and subscript L/R refers to left/right barrier. Here we assume that the bias voltage and temperature are so low as compared to the barrier height (~ 2 eV) that $|\mathcal{T}|^2$ can be assumed constant (and taken out from the integral) for electrons at all relevant microstates. The two electrodes are shifted with respect to each other by eV , the chemical potential difference, where V is the voltage applied across the junction. The net electrical current through the junction is

$$I = e(\Gamma_f - \Gamma_b). \quad (19)$$

At the end, one obtains

$$I = \frac{1}{eR_T} \int d\epsilon n_L(\epsilon) n_R(\epsilon + eV) [f_L(\epsilon) - f_R(\epsilon + eV)], \quad (20)$$

where R_T is the resistance of the tunnel barrier.

Problem 1.1: Obtain Eq. (20). Derive that the $I - V$ of a NIN (normal metal-insulator-normal metal) junction (see Fig. 4b) is ohmic $I = V/R_T$ at any temperatures T_L and T_R of the electrodes, even when $T_L \neq T_R$.

Tunneling rates for forward and backward processes of a NIN tunnel junction biased at voltage V for $T_L = T_R = T = (k_B\beta)^{-1}$ is given by

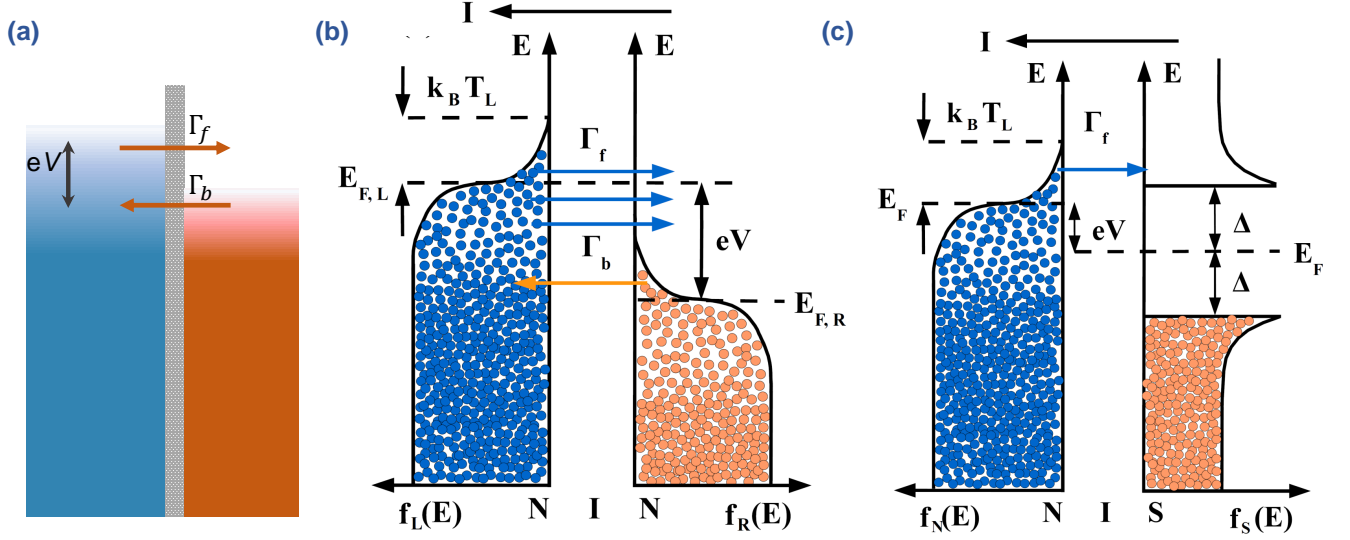


FIG. 4: Scheme of tunneling. (a) Generic with two electrodes separated by an insulating barrier. (b) Normal to normal tunneling. (c) Normal to superconductor tunneling.

$$\Gamma = \frac{1}{e^2 R_T} \frac{eV}{1 - e^{-\beta eV}}. \quad (21)$$

Problem 1.2: Obtain Eq. (21).

Next, we specify to an important setup for thermometry, a normal metal-insulator- superconductor NIS tunnel junction, as shown in Fig. 4a. In this case $n_L(\epsilon) = n_S(\epsilon)$ and $n_R(\epsilon) = 1$. We have then

$$I = \frac{1}{eR_T} \int d\epsilon n_S(\epsilon) [f_S(\epsilon) - f_N(\epsilon + eV)]. \quad (22)$$

Due to electron-hole symmetry the $I(V)$ is odd, $I(-V) = -I(V)$, and we obtain a symmetric form

$$I = \frac{1}{2eR_T} \int d\epsilon n_S(\epsilon) [f_N(\epsilon - eV) - f_N(\epsilon + eV)]. \quad (23)$$

This equation has an important message: the $I - V$ curve depends on the distribution, i.e. temperature in N, but not at all on that in the superconductor.

Problem 1.3: Show that for NIS junction at low temperatures, $eV, k_B T \ll \Delta$,

$$I = I_0 e^{-(\Delta - eV)/k_B T}, \quad (24)$$

with $I_0 \equiv \text{constant}$. This equation gives a primary temperature in the sense that

$$\frac{d}{dV} (\ln I) = \frac{e}{k_B T}, \quad (25)$$

where the slope is precisely $\frac{e}{k_B T}$, dictated just by constants of nature and temperature.

Problems 1.1-1.3: 2 points maximum.

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- [3] Francesco Giazotto, Tero T. Heikkilä, Arttu Luukanen, Alexander M. Savin, and Jukka P. Pekola, Opportunities for mesoscopics in thermometry and refrigeration: Physics and applications, Rev. Mod. Phys. **78**, 217 (2006).