The finite quantum grand canonical ensemble and temperature from single-electron statistics for a mesoscopic device

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Abstract. I present a theoretical model of a quantum statistical ensemble for which, unlike in conventional physics, the total number of particles is extremely small. The thermodynamical quantities are calculated by taking a small $N$ by virtue of the orthodicity of the canonical ensemble. The finite quantum grand partition function of a Fermi–Dirac system is calculated. The model is applied to a quantum dot coupled with a small two-dimensional electron system. Such a system consists of an alternatively singly and doubly occupied electron system confined in a quantum dot, which exchanges one electron with a small $N$ two-dimensional electron reservoir. The analytic determination of the temperature of a $(1 \leftrightarrow 2)$ electron system and the role of ergodicity are discussed. The generalized temperature expression in the small $N$ regime recovers the usual temperature expression form on taking the limit of $N \to \infty$ for the electron bath.

Keywords: mesoscopic systems (theory), quantum dots (theory), current fluctuations
1. Introduction

There is a deep connection between the nature of the elementary objects described by quantum mechanics and the emerging properties of thermodynamical quantities. Bohr clarified that the complementarity principle should apply to energy and temperature measurements. Indeed, the determination of the former is incompatible with knowledge of the latter when they refer to elementary objects [1]. After the creation of solid state quantum dots [2], it became possible to explore confined fermionic systems constituted of just a few electrons [3], down to a single localized electron [4]–[7]. Such systems are electrically probed by means of accurate charge sensing capable of determining current fluctuations corresponding to a variation of charge far below the charge unit [8]–[11]. The experimental determination of the electron temperature in a nanostructure is a difficult task [12], but it becomes a major issue when the system consists of a (1 ↔ 2) electron system in particle exchange with a few electron bath. Even if the definition of temperature $T = (\delta S/\delta U)^{-1}$ in terms of the energy $U$ and the entropy $S$ holds independently of the size of the ensemble [13], the systems considered here are far from bearing out the conventional assumptions for deriving thermodynamics from statistical physics. Apparently, it should not be possible to associate a temperature with such small systems. The reduction of the size of the system down to one electron in thermal and particle exchange with a finite electron system (small number of electrons $N$) implies a twofold change of perspective for determining the thermodynamical quantities. The first major change is the shift from space to time ensembles. Statistics can be recovered for a few particle open system only by considering the average of measurable quantities in the time domain. The second change consists in the generalization of the thermodynamics by removing the limit of large $N$, which implies that the terms at the order $1/N$ are relevant in the determination of the physical quantities. The equivalence under the first change of perspective is guaranteed by the ergodicity, while the second change is granted by the orthodicity. In section 2, I define the finite quantum grand partition ensemble in the limit of small $N$. Next, I determine the probability of occupation of an electronic system capable of containing either one or two electrons. The state equation is derived and it surprisingly depends on the heat capacity per area unit $c_A$. In section 3, the determination of the generalized...
temperature expression and its dependence from experimentally measurable quantities is described. Such evaluation is done by considering the realistic experimental condition of a single-electron quantum dot coupled with a small electron reservoir. The results are summarized and briefly discussed in section 4.

2. The finite quantum grand canonical ensemble of a $\left(1 \leftrightarrow 2\right)$ fermionic system

The grand canonical ensemble consists of a large open ensemble made of identical systems, which is in thermal equilibrium with a reservoir at a given temperature. The ensemble under investigation and the thermal reservoir may exchange energy and particles. In this section the statistical physics of a similar system is investigated. The model is derived for a generic system of fermions and it applies for electrons in a quantum dot. In contrast to the grand canonical ensemble case, here the open system under investigation may contain only one or two fermions. The reservoir is a low dimensional system of a few fermions. According to the physics and technology of semiconductor nanodevices, for which the present study is relevant, the reservoir is well approximated by a two-dimensional electron system (2DES), with a negligible extent in the direction perpendicular to the plane of the electrons [7,14]. To achieve uniformity of the notation, the island capable of capturing one extra electron is exemplified with a trap spatially extended along two dimensions, without any loss of generality. Such an assumption is realistic, the confinement of the electron wavefunction being symmetric in the $x$-$y$ plane both in defects at the Si/SiO$_2$ interface and in a quantum dot which is defined either lithographically or with a split gate in a heterostructure [14]. Therefore, all the definitions in the following refer to surfaces $\Sigma_i$ instead of volumes $V_i$ where $i = 1$ indicates the quantum dot and $i = 2$ a thermal bath made of $N_2$ electrons.

A system has orthodicity if the averages of the physical quantities over a given distribution recover the laws of thermodynamics. The canonical ensemble has native orthodicity, so such properties are present for the finite $N$ grand canonical ensemble by construction.

A given $H(N)$, the Hamiltonian of the system constituted by $N$ electrons distributed between the island and the 2DEG, can be separated as $H = H_1(N_1) + H_2(N_2)$ where $N_1 = 1, 2$.

Consequently one defines the finite quantum grand partition function for identical particles as follows:

$$Z(\Sigma, N, T) = \sum_{N_1=1}^{2} Z(\Sigma_1, N_1, T)Z(\Sigma_2, N_2, T)$$

$$= \sum_{N_1=1}^{2} \text{tr}(e^{-\beta H_1}) \text{tr}(e^{-\beta H_2})$$

where $N = N_1 + N_2$ and $\Sigma = \Sigma_1 + \Sigma_2$. We have introduced the function

$$\rho(N_1) = \frac{Z(\Sigma_2, N_2, T)}{Z(\Sigma_1 + \Sigma_2, N_1 + N_2, T)} e^{-\beta H_1(N_1)}$$
where $\beta = (kT)^{-1}$, which by definition satisfies
\begin{equation}
\sum_{N_1=1}^{2} \text{tr}(\rho(N_1)) = 1. \tag{4}
\end{equation}

Since $\text{tr}(\rho)$ is the canonical partition function times $Z(\Sigma_2, N_2, T)/Z(\Sigma, N, T)$, in the following such a ratio is calculated by means of the Helmholtz potential $\Psi = -\beta^{-1} \log Z$, which gives
\begin{equation}
\frac{Z(\Sigma_2, N_2, T)}{Z(\Sigma, N, T)} = e^{\beta \Psi(\Sigma_1 + \Sigma_2, N_1 + N_2, T) - \beta \Psi(\Sigma_2, N_2, T)}. \tag{5}
\end{equation}

In order to explicitly evaluate $\Psi$, the internal energy $U$ is now calculated, since $\Psi = U - TS = U + T(\delta S/\delta T)$ where $S = -(\delta \Psi/\delta T)$. Temperature $T$ is defined as usual using $T = (\delta S/\delta U)^{-1}$. For a Fermi 2DES of $M$ electrons in a surface with area $A$, in the limit of small temperature $T$, it holds that
\begin{equation}
U(M, A) = A \cdot u = A \left\{ \int_{\mu}^{\mu_F} E g(E) \, dE + \frac{\pi^2}{6} (k_B T)^2 [\mu g'(\mu) + g(\mu)] \right\}. \tag{6}
\end{equation}

\begin{equation}
M = A \cdot n = A \left\{ \int_{\mu}^{\mu_F} g(E) \, dE + \frac{\pi^2}{6} (k_B T)^2 [g'(\mu)] \right\}. \tag{7}
\end{equation}

where the density of states per surface unit is $g(E) \, dE = (m/\pi^2 \hbar^2) \, dE$ for a two-dimensional system with $d = 2$ and $\mu_F$ is the Fermi energy. Since $g'(E) = 0$ at $d = 2$,
\begin{equation}
U(M, A) = \frac{g}{2} A \mu_F^2 + \frac{\pi^2}{6} gA(k_B T)^2 \tag{8}
\end{equation}

\begin{equation}
M = gA \mu_F. \tag{9}
\end{equation}

The inversion of equation (9) gives the chemical potential
\begin{equation}
\mu(M, A) = \frac{M}{gA} \tag{10}
\end{equation}

so the internal energy $U$ can be equivalently written as
\begin{equation}
U(M) = \frac{1}{2} \frac{M^2}{gA} + \frac{\pi^2}{6} gA(k_B T)^2. \tag{11}
\end{equation}

The above relations are valid for $M = N_2$ electrons with $A = \Sigma_2$ and for $M = N_1 + N_2$ with $A = \Sigma_1 + \Sigma_2$, while $U(N_1)$ is treated separately because of the dependence of the nature of confinement when $N_1 = 1, 2$. The polynomial shape of $U(M) = a_{M,A} + b_A T^2$, where $a_{M,A} = \frac{1}{2}(M^2/gA)$ and $b_A = (\pi^2/6) gA(k_B)^2$, as a function of the temperature $T$ implies that $\Psi(M, A) = a_{M,A} - b_A T^2$, so
\begin{equation}
\Psi(M, A) = \frac{1}{2} \frac{M^2}{gA} - \frac{\pi^2}{6} gA(k_B T)^2. \tag{12}
\end{equation}
It is useful to calculate the heat capacity per area unit at constant surface area:

\[
c_A = \frac{1}{A} \left( \frac{\partial U(M,A)}{\partial T} \right)_A = \frac{\pi^2}{3} g k_B T, \tag{13}\n\]

and the pressure:

\[
P(M,A) = - \left( \frac{\partial \Psi(M,A)}{\partial A} \right)_T = \frac{1}{2} \frac{M^2}{g A^2} + \frac{\pi^2}{6} g (k_B T)^2. \tag{14}\n\]

Since the island which traps the electron has a very small spatial extent, the approximation \(\Sigma \approx \Sigma_2\) holds, which simplifies the analysis. It is now possible to evaluate the Helmholtz energy variation between \(N_1 + N_2\) and \(N_2\) electrons:

\[
\Delta \Psi = \Psi(N_1 + N_2, \Sigma_1 + \Sigma_2) - \Psi(N_2, \Sigma_2)
= \frac{(N_1 + N_2)^2}{2g(\Sigma_1 + \Sigma_2)} - \frac{N_2^2}{2g \Sigma_2} - \frac{\pi^2}{6} g (\Sigma_1 + \Sigma_2) (k_B T)^2 + \frac{\pi^2}{6} g \Sigma_2 (k_B T)^2 \tag{15}
\]

\[
\approx \frac{N_1^2 + 2N_1N_2 + N_2^2}{2g \Sigma_2} - \frac{N_2^2}{2g \Sigma_2} - \frac{\pi^2}{6} g \Sigma_1 (k_B T)^2 \tag{16}
\]

\[
= N_1 \mu(N_2, \Sigma_2) \left(1 + \frac{N_1}{2N_2}\right) - \frac{1}{2} c_A \Sigma_1 T. \tag{17}
\]

Putting \(\Delta \Psi\) in equation (5) gives

\[
\frac{Z(\Sigma_2, N - N_1, T)}{Z(\Sigma, N, T)} = e^{\beta \mu(N_2) N_1 (1 + (N_1/2N_2)) - c_A \Sigma_1 / 2k_B}. \tag{19}\n\]

The finite quantum grand canonical ensemble can therefore be defined via the pair \((E, \rho)\) with \(E = \Gamma\) and

\[
\rho(N_1) = z^{N_1(1+N_1/2N_2)} e^{-c_A \Sigma_1 / 2k_B} e^{-\beta H(N_1)} \tag{20}
\]

where \(z = e^{\beta \mu(N_2)}\), while \(\Gamma\) indicates all the states of the system over which the summations are performed and consists of the discrete quantum analogue of the Gibbs \(\Gamma\) space [15].

The probability of occupation of the subsystem 1 with \(L\) fermions is therefore

\[
p(L) = \frac{\text{tr} \rho(L)}{\sum_{N_1=1}^2 \text{tr}(\rho(N_1))} = \frac{z^{L(1+L/2N_2)} \text{tr}(e^{-\beta H_1(L)})}{\sum_{N_1=1}^2 z^{N_1(1+N_1/2N_2)} \text{tr}(e^{-\beta H_1(N_1)})} \tag{21}
\]

\[
= \frac{z^{L(1+L/2N_2)} \text{tr}(e^{-\beta H_1(L)})}{Z_{\text{QG}}} \tag{22}
\]

where

\[
Z_{\text{QG}} = \sum_{N_1=1}^2 z^{N_1(1+N_1/2N_2)} \text{tr}(e^{-\beta H_1(N_1)}). \tag{23}
\]

The present section is concluded by expressing the state equation and the relationship between the temperature \(T\) and the occupation statistics. Since \(\sum_{N_1=1}^2 \text{tr}(\rho(N_1)) = 1\), it
holds that
\[ Z_{QG} \cdot e^{-\left(c_A \sum_1 / 2k_B\right)} = 1 \] (24)
or, equivalently, if one considers the logarithm of both sides,
\[ \log Z_{QG} = \frac{c_A \sum_1}{2k_B} \] (25)

The generalized temperature of a \(1 \leftrightarrow 2\) system is therefore given by inversion:
\[ \frac{p(1)}{p(2)} = \frac{z^{1+(1/2N_2)} \text{tr}(e^{-\beta H_1(1)})}{z^{2(1+(1/N_2))} \text{tr}(e^{-\beta H_1(2)})}. \] (26)

In section 3 such a ratio is explicitly evaluated by considering a realistic value of a possible solid state quantum device.

3. The single-electron temperature in a quantum dot with a small \(N\) electron reservoir

In this section the physical parameters involved in the electron occupation probability of a realistic quantum dot and the consequent experimental determination of the generalized temperature are discussed. The study of the electron occupation of a quantum dot can be realized by measuring its charge state via the current in a channel electrically coupled to the electron charges confined to the dot [8, 16]. In the case of a natural quantum dot like a donor or a lattice point defect close to the Si/SiO\(_2\) interface, the channel is provided by the two-dimensional gas formed at the interface by applying a gate voltage [9, 11]. In the case of lithographically defined quantum dots, a current flows in the proximity of the island which confines the localized charges [14]. Let us consider as simple a system as we can, like a point defect close to the Si/SiO\(_2\) interface. Typically the 2DES is confined in \((50–300) \times (50–300) \text{ nm}^2\), while the electron wavefunction is spread along a few nm in the direction perpendicular to the 2DES [18]. The point defect can only accept one extra electron. When the defect is paramagnetic (it switches from \(N_1 = 1\) to 2 and vice versa), the first electron fills the ground state of a hydrogen-like shell, at energy \(E_1(1) = E_T\). Indeed, the high extraction energy of the unpaired electron makes it impossible to achieve the ionization of the first localized electron, unless a metal gate is used to manually modify the charge state from \(N_1 = 1\) to \(N_1 = 0\), which is not the case for the situation considered here. Because of the spin degeneracy, a second electron can be captured at the same energy level \(E_T\), to constitute a singlet state \(1/\sqrt{2}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)\), with two extra contributions due to the Coulomb charging energy \(\Delta E_C\) and to the lattice relaxation \(\Delta E_L\). While the origin of the first contribution is straightforward, the second requires a short discussion. The presence of the second electron involves in fact a rearrangement of the lattice [17]. At the low temperature considered here, the 2DES is weakly coupled with the crystal [19]. Phonons are involved in the emission and capture of one electron from the defect and the relaxation of the crystal implies a change of energy of \(S_{HR} \hbar \omega\) where \(S_{HR}\) is the Huang–Rhys factor and \(\omega\) is the average phonon frequency in the configuration coordinate picture [20]. In the following we consider \(\Delta E_L = S_{HR} \hbar \omega\), the energy gain of the lattice when an electron is captured. It is not possible for a natural quantum dot to capture a third electron because the energy of the system would exceed the conduction band edge energy.

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Figure 1. The change of the charge occupation, for both an artificial quantum dot and a natural point defect, is monitored by recording the sudden changes of an ultraweak channel current electrically coupled with it. The capture and the emission phenomena are generally governed by a Poisson process which determines the average occupation time. \( N_1 \) is the number of electrons in the dot. In this example the high current state is associated with the \( N_1 = 1 \) occupation. The two states could also be reversed (\( N_1 = 2 \) would refer to the high current state), depending on the microscopic nature of the electrostatic coupling of the island with the two-dimensional system.

The total energy of the two electrons is therefore

\[
E(2) = 2E_T + \Delta E_C + \Delta E_L.
\]  

(27)

Experimentally, the time resolved traces of the current are analysed by means of fast digitizers and they typically appear as random telegraph signals for both the quantum dots [16] and the point defects [10]. A typical switching current trace is shown in figure 1. The capture time \( \tau(1) \) and the emission time \( \tau(2) \) are obtained from averaging over thousands of switching events and they generally obey a Poissonian statistics. Deviations from such statistics are quantified by a non-unit Fano factor and they reflect quantum coherence typical of peculiarly coupled quantum dots [21]. Their ratio is governed by the ratio of the two occupation probabilities:

\[
\frac{\tau(1)}{\tau(2)} = \frac{p(1)}{p(2)}.
\]  

(28)

It is consequently appropriate to calculate the relative occupation probability for the two states with one or two electrons, since their ratio can be experimentally accessed. For the particular case discussed here, when the subsystem 1 is a paramagnetic point defect,

\[
\frac{p(1)}{p(2)} = 2e^{-\beta \mu (1+(3/2N_2))} \frac{e^{-\beta E_T}}{e^{-\beta E_T + \Delta E_C + \Delta E_L}}
\]  

(29)

\[
= 2e^{\beta(E_T + \Delta E_L + \Delta E_C - \mu(N_2)(1+(3/2N_2)))}.
\]  

(30)
The factor 2 takes into account the spin degeneracy of the ground state. The values of \( p(1) \) and \( p(2) \) are experimentally obtained as the average occupation times for the states 1 and 2 respectively. Such identification is possible by virtue of the ergodic hypothesis. The complete experimental determination of the parameters involved in equation (30) provides the generalized temperature \( T \) shared by the electrons in the quantum dot and the electrons in the 2DES. The generalized temperature of the electron(s) localized in the dots in thermal equilibrium with the small \( N_2 \)-electron bath may consequently be defined:

\[
T = k_B^{-1} \ln \frac{2 \tau(2)}{\tau(1)} \left( E_T + \Delta E_L + \Delta E_C - \mu(N_2) \left( 1 + \frac{3}{2N_2} \right) \right). \tag{31}
\]

It is remarkable that such a definition of the temperature of a time ensemble of a few electrons coincides with the usual one for a space ensemble just on taking \( N_2 \to \infty \). For this reason it can be considered a meaningful extension of the temperature definition for a small quantum system of electrons of the kind treated in the present paper. Such a result can be easily adapted to the case of the confinement induced in a artificial quantum dot, which does not require a lattice relaxation term.

4. Conclusion

The finite quantum grand canonical ensemble \((\mathcal{E}, \rho)\) has been defined for a fermionic system constituted by a cell capable of confining either one or two electrons, and a thermal bath of finite and small size made from a two-dimensional system of a few electrons. The state equation is governed by the heat capacity per unit surface \( c_A \) rather than the pressure. Averaging over a time ensemble replaces the average over space ensembles for the determination of the thermodynamical quantities. The ensemble approach has been applied for a quantum dot constituted by a natural point defect at the Si/SiO\(_2\) interface and it holds for a general \((1 \leftrightarrow 2)\) system. The ratio of the characteristic times monitored via the current two-state fluctuations is given by the ratio of the occupation probabilities calculated with the approach presented. Therefore, the generalized temperature of such a small time ensemble can be defined and extracted from the ratio of the average characteristic times of the two current states. Such a definition of temperature returns the usual temperature on taking the limit \( N \to \infty \) of the electron bath.

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