Exact canonical occupation numbers in a Fermi gas with finite level spacing and a $q$-analog of Fermi-Dirac distribution

Vyacheslavs Kashcheyevs
Faculty of Computing and Faculty of Physics and Mathematics,
University of Latvia, Riga LV-1586, Latvia
E-mail: slava@latnet.lv

Abstract. We consider equilibrium level occupation numbers in a Fermi gas with a fixed number of particles, $n$, and finite level spacing. Using the method of generating functions and the cumulant expansion we derive a recurrence relation for canonical partition function and an explicit formula for occupation numbers in terms of single-particle partition function at $n$ different temperatures. We apply this result to a model with equidistant non-degenerate spectrum and obtain close-form expressions in terms of $q$-polynomials and Rogers-Ramanujan partial theta function. Deviations from the standard Fermi-Dirac distribution can be interpreted in terms of a gap in the chemical potential between the particle and the hole excitations with additional correlations at temperatures comparable to the level spacing.
1. Introduction

Applications of statistical mechanics to fermion systems with discrete spectrum, such as semiconductor quantum dots [1, 2], naturally involve single-particle averages in statistical ensembles with a fixed number of particles. In particular, the kinetic theory of tunneling [3, 4] through quantum dots with fast intra-dot electron relaxation involves average level occupation number,

\[ \langle \nu_k \rangle_n = -\frac{1}{\beta Z_n} \frac{\partial Z_n}{\partial \epsilon_k}, \]

in a Gibbs distribution of \( n \) independent fermions populating a set of single-particle energy levels \( \{\epsilon_k\} \) (enumerated by \( k = 0, 1, 2 \ldots \)). Here \( Z_n \) is the canonical partition function

\[ Z_n = \sum_{\{\nu_k\}} \exp \left( -\beta \sum_k \nu_k \epsilon_k \right) \delta_{n, \sum_k \nu_k}, \]

and \( \beta \) is the inverse thermodynamic temperature. For fermions, occupation numbers \( \nu_k \) in the sum (2) take values 0 and 1.

The behavior of \( \langle \nu_k \rangle_n \) is simple in two extreme limits of the typical level \( \Delta \). For \( \beta \Delta \ll 1 \) and large \( n \), Eqs. (1)-(2) reduce to the standard Fermi-Dirac distribution,

\[ \langle \nu_k \rangle_n \rightarrow f(\epsilon_k - \mu) = \frac{1}{1 + e^{\beta(\epsilon_k - \mu)}}. \]

Here \( \mu \) is the chemical potential determined by the normalization condition \( n = \sum_k f(\epsilon_k - \mu) \). In the low temperature limit, \( \beta \Delta \gg 1 \), most of the statistical weight in Eq. (2) is in the ground state (defined as \( \nu_k = 1 \) for \( 0 \leq k < n \) and \( \nu_k = 0 \) otherwise). In this case it is common [5, 6] to take only one excited state into account resulting in a two-state Gibbs distribution which is equivalent to Eq. (3) for \( k = n-1, n \) with \( \mu = (\epsilon_n + \epsilon_{n-1})/2 \) and \( \beta \rightarrow \beta^* = 2\beta \).

For finite \( \beta \Delta \), the average occupation number \( \langle \nu_k \rangle_n \) deviates from Eq. (3) in a non-universal way which depends on the details of the energy spectrum [3, 7, 8]. Exact analytical investigation of this regime is complicated by the combinatorial explosion in the number of levels with comparable statistical weights. Particle number projection technique based on Fourier extraction [9, 7] gives an exact closed-form formula for \( \langle \nu_k \rangle_n \) (see Eq. (140) of [2]) that scales quadratically with the number of levels; however, its potential for analytical investigation appears to be limited due to the additional sum over the Fourier variable.

In the paper we address the problem of exact evaluation of canonical occupation numbers \( \langle \nu_k \rangle_n \) by deriving a general formula that scales linearly in the number of levels and quadratically in the number of particles, Eqs. (9) and (11) below. The energy spectrum \( \{\epsilon_k\} \) enters the formula only in terms of the single-particle partition function \( Z_1 \) computed at \( n \) different temperatures. We apply this general result to equidistant spectrum, \( \epsilon_k = k \Delta \), and derive an exact formula for \( \langle \nu_k \rangle_n \) in terms of polynomials in \( q = e^{-\beta \Delta} \), Eq. (14). In the limit of degenerate Fermi gas, \( n \beta \Delta \gg 1 \), these polynomials converge to partial theta function [10] which is involved in a number of combinatorial proofs [11, 12, 13] of Ramanujan’s identities [14]. The exact result for the equidistant spectrum can be approximated well by tailoring two standard Fermi-Dirac distributions [3] with different chemical potentials for holes and for particles, \( \mu_h = \epsilon_n \) and \( \mu_p = \epsilon_{n-1} \), respectively. In the high- and the low-temperature limits, this approximation converges to the asymptotically exact Fermi-Dirac and two-state
Gibbs distributions, respectively. At intermediate temperatures, $\beta \Delta \sim 1$, particle-hole correlation effects due to fixed $n$ result in finite deviations from the exact solution.

2. General expressions for fermion partition functions and the occupation numbers

Grand canonical partition function $Y$ serves as a generating function for the canonical partition functions $Z_n$ if expanded power series of $z = e^{\beta \mu_0}$,

$$Y(z) = \sum_{\{\nu_k\}} \exp\left(-\beta \sum_k \nu_k (\epsilon_k - \mu_0)\right) = 1 + \sum_{n=1}^\infty Z_n z^n. \tag{4}$$

$Y(z)$ is most conveniently calculated via its logarithm \cite{15},

$$\ln Y(z) = \sum_k \ln \left(1 + ze^{-\beta \epsilon_k}\right) = \sum_{n=1}^\infty \frac{\kappa_n}{n!} z^n, \tag{5}$$

where $\kappa_n \equiv (-1)^{n+1}(n-1)!Z_1(\beta n)$, and

$$Z_1(\beta') = \sum_k e^{-\beta' \epsilon_k} \tag{6}$$

is the canonical partition function of a single particle.

Relation between $n!Z_n$ and $\kappa_n$ is the same as between the raw moments and the cumulants of a univariate probability distribution and is given by the complete Bell polynomials \cite{16},

$$Z_n = (n!)^{-1} B(\kappa_1, \kappa_2, \ldots, \kappa_n). \tag{7}$$

The latter satisfy a recurrence relation \cite{17},

$$B(\kappa_1, \kappa_2, \ldots, \kappa_n) = \kappa_n + \sum_{m=1}^{n-1} \binom{n-1}{m-1} \kappa_m B(\kappa_1, \kappa_2, \ldots, \kappa_{n-m}), \tag{8}$$

which translates into

$$Z_n = \frac{1}{n} \sum_{m=1}^n (-1)^{m+1} Z_1(\beta m) Z_{n-m}. \tag{9}$$

We set $Z_0 = 1$ identically.

Combining Eqs. (1), (4) and (5) gives the generating function for the occupation numbers:

$$\sum_{n=1}^\infty \langle \nu_k \rangle_n Z_n z^n = Y(z) \frac{ze^{-\beta \epsilon_k}}{1 + ze^{-\beta \epsilon_k}}. \tag{10}$$

Expanding the r.h.s. in powers series in $z$ gives

$$\langle \nu_k \rangle_n = \frac{1}{Z_n^2} \sum_{m=1}^n (-1)^{m+1} e^{-\beta me_k} Z_{n-m}. \tag{11}$$

Equations (9) and (11) constitute our main general result.
3. Example: equidistant spectrum

3.1. Exact finite- \( n \) results: polynomials

For \( \varepsilon_k = k \Delta \), the grand canonical partition function \( Y(z) \) can be expressed by an infinite product,

\[
Y(z) = \prod_{k=0}^{\infty} (1 + q^k z) = (-z; q)_\infty, \tag{12}
\]

where \( q \equiv e^{-\beta \Delta} \) and \( (; q)_n \) is the \( q \)-shifted factorial \[18, 19\].

Using \( q \)-analog binomial theorem of Euler \[19\], formula 17.2.35) we can get the partition function directly from Eq. (4),

\[
Z_n = q^{n(n-1)/2} (q; q)_n. \tag{13}
\]

Applying Eq. (11), and transforming \( q \)-shifted factorials \[19\], formula 17.2.13), one gets

\[
\langle \nu_k \rangle_n = 1 - p(k, n; q), \tag{14}
\]

\[
p(k, n; q) = \sum_{m=0}^{n} q^{m(k+1)} (q^{-n}; q)_m
= 1 + \sum_{m=1}^{n} \prod_{l=0}^{m-1} (q^{k+1} - q^{l+k-n+1}). \tag{15}
\]

Equation (14) defines occupation numbers for \( n \) fermions populating equidistant levels at equilibrium. It is clear from the explicit form (16) that \( p(k, n; q) \) is a Laurent polynomial (the product contains negative powers of \( q \) if \( k < n \)). However, since \( 0 \leq \langle \nu_k \rangle_n \leq 1 \) for \( q \to 0 \) by definition (1), the negative powers of \( q \) must cancel, thus we conclude that \( p(k, n; q) \) is always an ordinary polynomial in \( q \) for \( n > 0, k \geq 0 \). This cancelation is not trivial and deems further mathematical investigation \[20\].

A number of recurrence formulas can be derived for \( p(k, n; q) \) \[21\], including a symmetry relation

\[
q^kp(k, n; q) = q^n p(n, k; q). \tag{17}
\]

Using (16) in the r.h.s. of (17) gives a sum of products with no negative powers of \( q \) at \( k < n \).

3.2. Large- \( n \) limit: \( q \)-analog of Fermi-Dirac distribution

If \( \varepsilon_n \gg \beta^{-1} \) then the Fermi gas is degenerate \[15\] and the limit of \( q^n \to 0 \) is appropriate. For \( k, n \to \infty \), and \( k - n = \text{const} \geq -1 \) the polynomial sum in Eq. (16) becomes a geometric series which gives

\[
\lim_{k \to n-1} p(k, n; q) = \theta(-q^{k-n+1/2}, q^{1/2}), \tag{18}
\]

where

\[
\theta(a, q) = \sum_{m=0}^{\infty} a^m q^m \tag{19}
\]
is known as partial theta function\textsuperscript{†} \cite{10}. The partial theta function is famous for a number of identities discovered by Ramanujan in his lost notebook \cite{14}. These identities have been studied extensively \cite{22, 10}, including some recent proofs by combinatorial methods \cite{11, 12, 13}. Using the symmetry relation (17) for $k < n$, gives the particle-hole complementary result: \( \lim_{n \to \infty} p(k, n; q) = 1 - \theta(-q^{n-k-1/2}, q^{1/2}) \).

In terms of level energies $\epsilon_k$, the occupation numbers in a canonical degenerate Fermi gas with constant levels spacing $\Delta$ can be written as

\[
\lim_{n \to \infty} \langle \nu_k \rangle_n = \begin{cases} 
  f_q(\epsilon_k - \mu + \Delta/2), & \epsilon_k > \mu + \Delta/2, \\
  1 - f_q(-\epsilon_k + \mu + \Delta/2), & \epsilon_k < \mu - \Delta/2,
\end{cases} \tag{20}
\]

where

\[
f_q(\epsilon) = \theta(-e^{-\beta\epsilon}, q^{1/2}) \overset{q \to 1}{=} f(\epsilon).
\]

and $\mu = (\epsilon_n + \epsilon_{n-1})/2$. The function defined in Eq. (20) can be considered a $q$-analog \cite{18} of the standard Fermi-Dirac distribution \cite{3} since $\lim_{q \to 1} f_q(\epsilon) = f(\epsilon)$.

Equation (20) expresses two essential deviations of canonical occupation numbers from Fermi-Dirac distribution. Firstly, the $q$-analog $f_q$ is different from $f$. An approximation of substituting $f_q \to f$ in Eq. (20) becomes exact both for $q \to 1$ and for $q \to 0$. Numerically, we find maximal absolute deviation $|f(\epsilon_k) - f_q(\epsilon_k)|$ of 0.0567 reached for $k = n, n-1$ at $\beta\Delta = 0.752$. For the two levels closest to the gap, $k = n-1, n$ approximating $f_q \to f$ gives $\langle \nu_n \rangle_n = 1 - \langle \nu_{n-1} \rangle_n = \exp(-\beta\Delta/2)/(2 \cosh(\beta\Delta/2))$ which is equivalent to two-state Gibbs approximation \cite{3}. A comparison between the exact

\[\text{Note that } \lim_{n \to \infty} p(n, n; q) = \sum_{m=0}^{\infty} (-1)^m q^m (m+1)/2 \text{ is an instance of } false \text{ theta series} \text{ \cite{22} in the sense of L. J. Rogers \cite{23}.}\]
result (14), the large-$n$ limit (20) and a single Fermi-Dirac distribution is shown in Fig. 1 for $n = 4$ and $\beta \Delta = 1$.

Secondly, barring the difference between $f_q$ and $f$, Eq. (20) can be seen as a combination of two Fermi-Dirac distributions with different chemical potentials for particles, $\mu_p = \mu - \Delta/2 = \epsilon_{n-1}$, and for holes, $\mu_h = \mu + \Delta/2 = \epsilon_n$, respectively. This is precisely what is to be expected if one considers particle and hole excitations from the ground state as two uncorrelated microcanonical ensembles. In this view, the moderate difference in the functional dependence between $f(\epsilon)$ and $f_q(\epsilon)$ results from correlation between a particle and a hole created in a single pair-excitation act. Note that the difference $\mu_h - \mu_p = \Delta$ can not be ignored even as $\beta \to \infty$ and $q \to 0$, thus using a single Fermi-Dirac distribution, Eq. (3), necessarily fails for finite $\Delta$ and low temperature.

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