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LETTER TO THE EDITOR

Fermions in finite canonical ensembles: comparison between two formalisms

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Abstract. Occupancies in certain small, electrically insulated, electron systems have been recently calculated. We show that the recursive formula derived from second quantization and the simple expression obtained from combinatorics are identical.

As a consequence of the recent availability of electron traps and the tendency to fabricate smaller and smaller electronic devices, there is a growing interest in the quantum statistics of finite (i.e. small) electron systems. When the system may exchange energy (heat), but not electrons, with a substrate, the celebrated Fermi–Dirac distribution only applies in the large-temperature limit. Otherwise, significant discrepancies occur.

In this paper I restrict myself to evenly spaced one-electron energy levels, $\varepsilon_k = k\varepsilon$, where the energy spacing ε is a constant, $k \in \mathbb{Z}$, and $k = 0$ labels the top electron location at $T = 0$ K. A single-electron spin-state is considered.

An expression for the level occupancy $N_k(q)$ of level k, where $q \equiv \exp(-\varepsilon/k_B T)$ is the Boltzmann factor, was apparently first obtained by Schonhammer and Meden [1] from second quantization of the electron wavefunction. Occupancies are the coefficients of the Laurent series

$$\sum_{k\in\mathbb{Z}} N_k(q) z^k = \left(\sum_{\ell\geqslant 0} \frac{1}{z^\ell}\right) \frac{F(z)F(\frac{1}{z})}{F(1)^2} \tag{1}$$

where

$$F(z) = \exp\left(\sum_{n\geqslant 1} \frac{z^n}{n(q^{-n}-1)}\right). \tag{2}$$

Shortly thereafter, Arnaud and others [2] obtained a much simpler, explicit expression, by direct enumeration of the microstates followed by averaging. Their result reads

$$N_k(q) = \sum_{i\geqslant 0} (-1)^i q^{(i+1)k+\frac{i(i+1)}{2}}. \tag{3}$$

The purpose of this paper is to show that equations (1) and (3) coincide. The proof involves elementary theorems on q-series. It thus appears that the second-quantization methods are often superfluous. Our direct approach (see [2,3]) may be greatly generalized, e.g., to arbitrary level degeneracies, and is capable of solving problems that could be very difficult to solve by other methods.

The first task is to expand $F(z)$ defined in (2) in power series of z. We have

$$F(z) = \exp\left(\sum_{n>0}\frac{(zq)^n}{n}\sum_{i\geqslant 0}q^{ni}\right) = \exp\left(-\sum_{i\geqslant 0}\ln(1-zq^{i+1})\right) = \frac{1}{(zq)_\infty} = \sum_{m\geqslant 0}\frac{q^m}{(q)_m}z^m \tag{4}$$

where the notations

$$(a)_\infty = \prod_{i\geqslant 0}(1-aq^i) \qquad \text{and} \qquad (a)_m = \frac{(a)_\infty}{(aq^m)_\infty}$$

have been used. In particular, $F(1) = 1/(q)_\infty$. In the last step in (4), a theorem of Cauchy, recalled in the appendix, has been employed.

Introducing the power series expansion of $F(z)$ into the right-hand side of (2), we obtain

$$\left(\sum_{\ell\geqslant 0}\frac{1}{z^\ell}\right)\frac{F(z)F(\frac{1}{z})}{F(1)^2} = (q)_\infty^2\sum_{\ell\geqslant 0}\sum_{m\geqslant 0}\sum_{n\geqslant 0}\frac{q^{m+n}z^{m-n-\ell}}{(q)_m(q)_n}. \tag{5}$$

Observe that the index m in the above sum may run from any negative integer, because $1/(q)_m$ vanishes for negative m. Collecting terms of power z^k in the right-hand side of (5), the occupancy of level k reads

$$N_k(q) = (q)_\infty^2\sum_{\ell\geqslant 0}\sum_{n\geqslant 0}\frac{q^{2n+\ell+k}}{(q)_{n+\ell+k}(q)_n}.$$

A formula of Heine, also recalled in the appendix, enables us to simplify the above expression to

$$N_k(q) = \sum_{i\geqslant 0}(-1)^i q^{(i+1)k+\frac{i(i+1)}{2}}$$

which is equation (3).

Appendix

The two formulae employed in the main text, namely in equations (4) and (5), are special forms of the two following identities, which are due to Cauchy and Heine, respectively. Proofs can be found, e.g., in [4] (theorem 2.1 and corollary 2.3). For $|q| < 1$, $|t| < 1$, and $|b| < 1$,

$$\sum_{n\geqslant 0}\frac{(a)_n}{(q)_n}t^n = \frac{(at)_\infty}{(t)_\infty}$$

and

$$\sum_{n\geqslant 0}\frac{(a)_n(b)_n}{(q)_n(c)_n}t^n = \frac{(b)_\infty(at)_\infty}{(c)_\infty(t)_\infty}\sum_{n\geqslant 0}\frac{(c/b)_n(t)_n}{(q)_n(at)_n}b^n.$$

Letting $a = 0$ and $b \to 0$ in Heine's formula, we obtain

$$\sum_{n\geqslant 0}\frac{t^n}{(q)_n(c)_n} = \frac{1}{(c)_\infty(t)_\infty}\sum_{n\geqslant 0}(-1)^n\frac{(t)_n}{(q)_n}q^{\binom{n}{2}}c^n.$$

Therefore,

$$\sum_{n\geqslant 0} \frac{q^{2n}}{(q)_n (q^{\ell+k+1})_n} = \frac{1}{(q^{\ell+k+1})_\infty (q^2)_\infty} \sum_{n\geqslant 0} (-1)^n \frac{(q^2)_n}{(q)_n} q^{\frac{n(n-1)}{2}+n(\ell+k+1)}$$
$$= \frac{(q)_{\ell+k}}{(q)_\infty^2} \sum_{n\geqslant 0} (-1)^n (1-q^{n+1}) q^{\frac{n(n+1)}{2}+n(\ell+k)}.$$

Finally,

$$N_k(q) = (q)_\infty^2 \sum_{\ell\geqslant 0} \frac{q^{\ell+k}}{(q)_{\ell+k}} \sum_{n\geqslant 0} \frac{q^{2n}}{(q)_n (q^{\ell+k+1})_n} = \sum_{n\geqslant 0} (-1)^n q^{\frac{n(n+1)}{2}+(n+1)k}.$$

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