

Partitions and the Fermi–Dirac Distribution

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The exact electron distribution in certain small isolated systems is derived from the enumeration of the partitions of integers. The corresponding generating series are ascribed a physical interpretation. The well-known Fermi–Dirac statistics is recovered by averaging. © 2000 Academic Press

1. INTRODUCTION

For systems of electrons that can exchange energy and particles with a large medium, the celebrated Fermi–Dirac (FD) distribution provides the probability for an electron to occupy a given energy level after the total energy of the system has been increased. This powerful tool derives from the laws of statistical mechanics (see, e.g., Landau and Lifchitz [3]). But this result does not apply to small isolated systems. Arnaud *et al.* [2] propose to compute the exact distribution in such systems by direct enumeration. This is done in the present paper, with the help of certain partitions of integers.

The systems considered are isolated and one-dimensional with evenly spaced energy levels (the spacing is conveniently assumed to be unity). Two electrons cannot occupy the same level according to the Pauli exclusion principle, the electron spin being presently ignored. Figure 1 shows the initial (zero temperature) configuration of the system ($n=0$), and the possible configurations (microstates) after an increase of the energy by $n=3$ and $n=6$ units. The total number N of electrons of the system is assumed to be larger than n , and the energy levels are indexed by the integer k , with $k=0$ labeling the electron on top of the initial configuration.

The number of microstates for a given integral value n of added energy is the number $p(n)$ of partitions of n (for references to the theory of partitions, see, e.g., Andrews [1]). In the physical model, the microstates are assumed to be equally likely. The desired probability follows from the computation of the number $m(n, k)$ of microstates that exhibit an electron at

k	$m(0, k)$	$m(3, k)$		$m(6, k)$
7	0	0		0
6	0	0	•	1
5	0	0	•	1
4	0	0	• •	2
3	0	•	1 • • •	3
2	0	•	1 • • • •	4
1	0	•	1 • • • • •	5
0	•	1 • •	2 • • • • • •	6
-1	•	1 • •	2 • • • • • •	7
-2	•	1 • •	2 • • • • • •	8
-3	•	1 • • •	3 • • • • • •	9
-4	•	1 • • •	3 • • • • • •	10
-5	•	1 • • •	3 • • • • • •	10
-6	•	1 • • •	3 • • • • • •	11
	$n = 0$	$n = 3$		$n = 6$

FIG. 1. $N=7$.

level k after the energy has been increased by n units. The main purpose of this paper is to derive an expression for $m(n, k)$. Section 2 describes some useful sets of partitions. Several formulas in Section 3 link the numbers $m(n, k)$ with the numbers $p(n)$. We also derive the number $m(n; k; k')$ of microstates that exhibit one electron at level k and none at level k' . Section 4 is devoted to some physical applications. The Fermi–Dirac distribution follows from the previous considerations through averaging with respect to n and with respect to N .

2. PARTITIONS

In this paper, a *partition* of an integer n is agreed to be a *non-increasing* infinite sequence of nonnegative integers summing up to n . Such a sequence

$$(a_1, a_2, \dots), \quad \text{with } a_i \in \mathbb{N}, \quad a_1 \geq a_2 \geq \dots, \quad \text{and} \quad \sum_{i \geq 1} a_i = n,$$

is also denoted by \mathbf{a} or (a_i) ; the positive terms of a partition \mathbf{a} are called its *parts*, and the *length* of \mathbf{a} is the number of its parts.

Let $\mathbf{P}(n)$ be the set of all partitions of n , its cardinal $|\mathbf{P}(n)|$ is usually denoted by $p(n)$. Note that the mapping p is defined on \mathbb{Z} , and that $p(0) = 1$ and $p(n) = 0$ if $n < 0$. Various expressions of the (ordinary) generating series Gp of the $p(n)$'s are known. For $n \in \mathbb{N}$ and fixed $|q| < 1$, we use the notations

$$(a)_0 = 1, \quad (a)_n = \prod_{i=0}^{n-1} (1 - aq^i), \quad \text{and} \quad (a)_\infty = \lim_{n \rightarrow \infty} (a)_n,$$

$\mathbf{P}(n)$	$\tau_n(\mathbf{P}(n))$	$\epsilon_n(\mathbf{P}(n))$
$(4,0,\dots)$	$(8,3,2,1,0,\dots)$	$(1,1,1,0,0,0,0,1)$
$(3,1,0,\dots)$	$(7,4,2,1,0,\dots)$	$(1,1,0,1,0,0,1,0)$
$(2,2,0,\dots)$	$(6,5,2,1,0,\dots)$	$(1,1,0,0,1,1,0,0)$
$(2,1,1,0,\dots)$	$(6,4,3,1,0,\dots)$	$(1,0,1,1,0,1,0,0)$
$(1,1,1,1,0,\dots)$	$(5,4,3,2,0,\dots)$	$(0,1,1,1,1,0,0,0)$

FIG. 2. Representations for $n = 4$.

and we have

$$Gp(q) = \sum_{n \geq 0} p(n) q^n = \frac{1}{(q)_\infty}.$$

Let x^+ stand for $\max(x, 0)$. We first define a mapping τ_n from $\mathbf{P}(n)$ to $\mathbb{N}^{\mathbb{N}^*}$ by

$$\tau_n((a_i)) = (a_i + (n + 1 - i)^+).$$

For positive n , this mapping generates an “electronic” representation ϵ_n of the elements of $\mathbf{P}(n)$ in the following way: Denoting by $\binom{n+1}{2}$ the triangular number $n(n+1)/2$, it is easy to check that $\tau_n(\mathbf{P}(n)) \subseteq \mathbf{P}(n + \binom{n+1}{2})$. Then we define the mapping ϵ_n from $\mathbf{P}(n)$ to $\{0, 1\}^{2n}$ by

$$\epsilon_n(\mathbf{a}) = v, \quad \text{with } (v_i = 1 \iff \exists j \geq 1, i = \tau_n(\mathbf{a})_j) \quad \text{for each } i \in 1 \cdots 2n.$$

An example ($n = 4$) is shown in Fig. 2.

We primarily aim to compute the vertical marginal values in the $\{0, 1\}$ -matrix displayed in Fig. 2, which are precisely the $m(n, k)$ ’s for $k = (1 - n) \cdots n$. For example, $(m(4, k))_{k=-3 \cdots 4} = (4, 4, 3, 3, 2, 2, 1, 1)$. Notice that, for positive k , $m(n, k)$ is the number of partitions of n that contain either k as the first term or $k + 1$ as the second term, etc.

LEMMA 1. *Let n be a positive integer. The mapping τ_n is one-to-one, onto the set of all partitions of $n + \binom{n+1}{2}$ with exactly n distinct parts taken in $1 \cdots 2n$. The mapping ϵ_n is one-to-one, onto the set of all vectors v in $\{0, 1\}^{2n}$ such that*

$$\sum_{i=1}^{2n} v_i = n, \quad \text{and} \quad \sum_{i=1}^{2n} i v_i = n + \binom{n+1}{2}. \tag{1}$$

Proof. The mapping τ_n is clearly one-to-one. Moreover, if $\mathbf{b} = \tau_n(\mathbf{a})$ with $\mathbf{a} \in \mathbf{P}(n)$ then

$$b_1 = a_1 + n \leq 2n,$$

$$b_n = a_n + 1 > 0,$$

$$b_{n+1} = 0,$$

$$b_i - b_{i+1} = a_i - a_{i+1} + 1 > 0 \quad \text{for } i = 1 \dots (n-1).$$

Thus the length of \mathbf{b} is n ; its parts are pairwise distinct and do not exceed $2n$. Conversely, let \mathbf{b} be a partition of $n + \binom{n+1}{2}$ with exactly n distinct parts taken in $1 \dots 2n$, and let $a_i = b_i - (n+1-i)^+$. It is easily checked that (a_i) is non-increasing and lies in $\mathbf{P}(n)$, and that $\mathbf{b} = \tau_n((a_i))$.

Now, ε_n is one-to-one since partitions in $\tau_n(\mathbf{P}(n))$ have distinct parts. Its range, according to the range of τ_n , is contained in the set of all vectors v of $\{0, 1\}^{2n}$ for which (1) holds.

Conversely, let v be such a vector and let $(a_i)_{i=1 \dots 2n}$ be the (unique) non-increasing sequence obtained by reindexing the sequence $(iv_i)_{i=1 \dots 2n}$. Then $(a_i)_{i=1 \dots 2n}$ may be considered as an element \mathbf{a} of $\mathbf{P}(n + \binom{n+1}{2})$. It is easily seen that \mathbf{a} lies in $\tau_n(\mathbf{P}(n))$, and that $v = \varepsilon_n(\tau_n^{-1}(\mathbf{a}))$. ■

Given any integers k and n , we formally define now $m(n, k)$ as the number of sequences in $\tau_n(\mathbf{P}(n))$ that contain the term $(n+k)^+$. These numbers $m(n, k)$ are precisely those mentioned in the Introduction: of course, $m(n, k) = p(n)$ if $k \leq -n \leq 0$ (since each partition contains the term 0), and $m(n, k) = 0$ if either $n < 0$ (since $\mathbf{P}(n)$ is empty) or $k > n \geq 0$ (since the terms of any partition in $\tau_n(\mathbf{P}(n))$ do not exceed $2n$). Moreover, for $-n < k \leq n$ the number $m(n, k)$ is exactly the number of vectors in $\varepsilon_n(\mathbf{P}(n))$ whose $(n+k)$ th component equals 1.

Let us finally exhibit subsets of $\mathbf{P}(n)$ that will be useful in what follows, and give some of their basic properties. Let n and k be any integers, and let $j \geq 1$, and denote by $\mathbf{P}(n, k, j)$ the set of all partitions of n that contain k as j th term, i.e.,

$$\text{for } j \geq 1, \quad \mathbf{P}(n, k, j) = \{\mathbf{a} \in \mathbf{P}(n) : a_j = k\}.$$

Notice that $\mathbf{P}(n, k, j) \neq \emptyset$ if, and only if, the inequalities $0 \leq kj \leq n$ hold. Let us now define, for *positive* k ,

$$\mathbf{M}(n, k) = \bigcup_{j \geq 1} \mathbf{P}(n, k + j - 1, j).$$

LEMMA 2. *The sets $\mathbf{M}(n, k)$ satisfy*

$$(i) \quad \mathbf{M}(n, k) \neq \emptyset \iff k \leq n.$$

(ii) $\mathbf{M}(n, k) = \bigcup_{j \geq 1} \mathbf{P}(n, k + j - 1, j)$, a finite disjoint union.

Proof. (i) $\mathbf{M}(n, k) \neq \emptyset \Leftrightarrow \exists j \geq 1, kj + j(j - 1) \leq n \Leftrightarrow k \leq n$.

(ii) On the one hand, the union is disjoint because partitions are non-increasing sequences. On the other hand, it is finite since values $j \geq \frac{1}{2}(1 - k + \sqrt{(k - 1)^2 + 4n})$ force $\mathbf{P}(n, k + j - 1, j) = \emptyset$. ■

As noticed above, the cardinality of $\mathbf{M}(n, k)$ is $m(n, k)$, for positive k .

LEMMA 3. For all integers n and all positive integers k , $m(n, k) = |\mathbf{M}(n, k)|$.

Proof. According to Lemma 2, equality holds if either $n < 0$ or $k > n \geq 0$. Let $0 < k \leq n$ and $\mathbf{a} \in \tau_n(\mathbf{P}(n))$, then $\mathbf{a} \in \tau_n(\mathbf{M}(n, k))$ if and only if there exists $i \geq 1$ such that

$$a_i = (k + i - 1) + n + 1 - i = k + n.$$

Therefore, $m(n, k) = |\tau_n(\mathbf{M}(n, k))| = |\mathbf{M}(n, k)|$ by Lemma 1. ■

3. FORMULAS

First notice that only positive values of k are to be considered because of the following symmetry:

PROPOSITION 1. For each integer k ,

$$m(n, -k) + m(n, k + 1) = p(n). \tag{2}$$

Proof. First assume $k \geq 0$. According to the above discussion, $k \geq n \geq 0$ yields $m(n, k + 1) = 0$ and $m(n, -k) = p(n)$. Moreover, both members in (2) vanish for $n < 0$. Thus we may assume $k < n$. Consider the involution π defined on $\{0, 1\}^{2n}$ by complementation and reversion:

$$\pi((v_1, \dots, v_{2n})) = (1 - v_{2n}, \dots, 1 - v_1).$$

Clearly, π is a permutation of $\varepsilon_n(\mathbf{P}(n))$. Now, let $\mathbf{a} \in \mathbf{P}(n)$; $\tau_n(\mathbf{a})$ contains the part $(n - k)$ if and only if $\varepsilon_n(\mathbf{a})_{n-k} = 1$, which is equivalent to $\pi(\varepsilon_n(\mathbf{a}))_{n+1+k} = 0$, which amounts to saying that $\varepsilon_n^{-1}(\pi(\varepsilon_n(\mathbf{a})))$ is not in $\mathbf{M}(n, 1 + k)$. Therefore,

$$m(n, -k) = |\mathbf{P}(n) \setminus \mathbf{M}(n, k + 1)| = p(n) - m(n, k + 1).$$

Finally, for negative k , turn k into $-k - 1$ to complete the proof. ■

Incidentally, the mapping π defined above corresponds with the usual conjugation in $\mathbf{P}(n)$. The formal proof is omitted. As a first consequence of Proposition 2, we next show that $p(n)$ is linked with the numbers $m(n, k)$, for positive k , in the following way:

COROLLARY 1. For $n > 0$,

$$p(n) = \frac{1}{n} \sum_{k=1}^n (2k-1) m(n, k). \quad (3)$$

Proof. According to Lemma 1 and relation (2) we have

$$\begin{aligned} (n + \binom{n+1}{2}) p(n) &= \sum_{v \in \varepsilon_n(\mathbf{P}(n))} \sum_{1 \leq i \leq 2n} i v_i = \sum_{1 \leq i \leq 2n} i \sum_{v \in \varepsilon_n(\mathbf{P}(n))} v_i \\ &= \sum_{1 \leq i \leq 2n} i m(n, i-n) = \sum_{1-n \leq k \leq n} (n+k) m(n, k) \\ &= \sum_{1-n \leq k \leq 0} (n+k) [p(n) - m(n, 1-k)] \\ &\quad + \sum_{1 \leq k \leq n} (n+k) m(n, k) \\ &= \binom{n+1}{2} p(n) + \sum_{1 \leq k \leq n} (2k-1) m(n, k). \quad \blacksquare \end{aligned}$$

With the help of the second relation in Lemma 2, the numbers $m(n, k)$ for positive k can be obtained from the numbers $p(n, k, j) = |\mathbf{P}(n, k, j)|$ through the (finite) sum

$$m(n, k) = \sum_{j \geq 1} p(n, k + j - 1, j).$$

Indeed, the generating series of the $p(n, k, j)$'s for fixed k and j is given by

PROPOSITION 2.

$$\sum_{n=-\infty}^{\infty} p(n, k, j) q^n = \sum_{n \geq kj} p(n, k, j) q^n = \frac{q^{kj}}{(q)_k (q)_{j-1}}.$$

Proof. Let $\mathbf{a} \in \mathbf{P}(n)$ with $a_j = k$, the Ferrers graph of \mathbf{a} has the form given in Fig. 3.

Given i such that $\mathbf{P}(n, k+i-1, i) \neq \emptyset$, let ϕ_i be the mapping from $\mathbf{P}(n, k+i-1, i)$ to $\mathbf{P}(n-k)$ defined by

$$\phi_1((k, a_2, a_3, \dots)) = (a_2, a_3, \dots),$$

$$\phi_i((a_1, \dots, a_{i-1}, k+i-1, a_{i+1}, \dots)) = (1+a_1, \dots, 1+a_{i-1}, a_{i+1}, \dots) \quad \text{if } i > 1.$$

Notice that, given any $j \geq 1$, the range of ϕ_i does not intersect the set

$$\mathbf{P}(n-k, k+j, j) = \{\mathbf{b} \in \mathbf{P}(n-k) : b_j = k+j\}.$$

Indeed, let $\mathbf{a} \in \mathbf{P}(n, k+i-1, i)$ and $\mathbf{b} = \phi_i(\mathbf{a})$. We have

$$\text{for } j < i, \quad b_j = 1 + a_j \geq 1 + a_i = k+i > k+j,$$

and

$$\text{for } j \geq i, \quad b_j = a_{j+1} \leq k+i-1 < k+j.$$

Therefore, by Lemma 2,

$$\phi_i(\mathbf{P}(n, k+i-1, i)) \cap \mathbf{M}(n-k, k+1) = \emptyset;$$

thus, by Lemma 2 again, a mapping ϕ from $\mathbf{M}(n, k)$ to $\mathbf{P}(n-k)$ may be defined by

$$\phi(\mathbf{a}) = \phi_i(\mathbf{a}) \quad \text{if } \mathbf{a} \in \mathbf{P}(n, k+i-1, i),$$

that satisfies $\phi(\mathbf{M}(n, k)) \cap \mathbf{M}(n-k, k+1) = \emptyset$. Each ϕ_i is clearly one-to-one. Moreover, if $\mathbf{a} \in \mathbf{P}(n, k+i-1, i)$ and $\mathbf{a}' \in \mathbf{P}(n, k+j-1, j)$ with $i < j$ then the equality $\phi(\mathbf{a}) = \phi(\mathbf{a}')$ implies

$$k+i-1 = a_i \geq a_{i+1} = 1+a'_i \geq 1+a'_j > a'_j = k+j-1,$$

a contradiction, so that ϕ is one-to-one, too.

To obtain the desired formula, it suffices then to show that each element \mathbf{b} of the set $\mathbf{P}(n-k) \setminus \mathbf{M}(n-k, k+1)$ lies in the range of ϕ . Since (b_i) is non-increasing, the set $\{i \in \mathbb{N} : b_i < i+k\}$ is not empty; j standing for its smallest element, let \mathbf{a} be the sequence defined as follows:

$$a_j = k+j-1,$$

$$a_i = b_{i-1} \quad \text{for all } i > j$$

$$\text{if } j > 1, \quad a_i = b_i - 1 \quad \text{for all } i \in 1 \cdots (j-1).$$

On the one hand, \mathbf{a} is non-increasing: first, $a_j = k+j-1 \geq b_j = a_{j+1}$; second, if $j > 1$ then $b_{j-1} \geq k+j-1$ by definition of j , thus $b_{j-1} \geq k+j$

since $\mathbf{b} \notin \mathbf{P}(n-k, k+j, j-1)$, thus $a_{j-1} = b_{j-1} - 1 \geq a_j$. On the other hand, by construction of \mathbf{a} , its terms sum up to n and $\mathbf{b} = \phi(\mathbf{a})$. ■

Remark. It must be noticed that, in the latter proof, the partition $\phi(\mathbf{a})$ of $n-k$ has exactly one part less than the partition \mathbf{a} of n . This seemingly innocuous fact would allow us to get rid of the assumption $N \geq n$. Indeed, assume $N < n$. The number of possible microstates is then the cardinality $p_N(n)$ of the set $\mathbf{P}_N(n)$ of all partitions of n with at most N parts (since only N electrons are available). Denoting by $m_N(n, k)$ the cardinality of $\mathbf{M}(n, k) \cap \mathbf{P}_N(n)$, we get the relation

$$m_N(n, k) = p_{N-1}(n-k) - m_{N-1}(n-k, k+1). \tag{5}$$

As a consequence of Theorem 1, the numbers $m(n, k)$ are easily computed with the help of the following formula, which provides us with a generating series Gm_k for fixed k :

COROLLARY 2. *For all $k \in \mathbb{Z}$ and $n > 0$, $\binom{i+1}{2}$ standing for the i th triangular number $\frac{i(i+1)}{2}$,*

$$m(n, k) = \sum_{i \geq 0} (-1)^i p(n - \binom{i+1}{2} - (i+1)k). \tag{6}$$

Moreover, with the further notation $T_k(q) = \sum_{n \geq 0} (-1)^n q^{\binom{n+1}{2} + nk}$,

$$Gm_k(q) = \sum_{n \geq 0} m(n, k) q^n = \frac{q^{k^+}}{(q)_\infty} T_{|k|}(q). \tag{7}$$

Proof. Note that the sum in (6) is finite, since $p(j)$ vanishes for negative j . For positive k , the formula easily follows from (4). For non-positive k we have

$$\begin{aligned} & \sum_{i \geq 0} (-1)^i p(n - \binom{i+1}{2} - (i+1)k) \\ &= \sum_{i \geq 2k-1} (-1)^{i+1} p(n - \binom{i+1}{2} - (i+1)(-k+1)). \end{aligned}$$

In the latter expression, the sum for i from $2k-1$ to -2 vanishes (change i into $2k-3-i$), the term for $i = -1$ is $p(n)$, and the remaining sum is $-m(n, 1-k)$. According to Proposition 2, the proof of (6) is complete. Furthermore, (6) immediately leads to the generating series

$$\sum_{n \geq 0} m(n, k) q^n = \sum_{n \geq 0} p(n) q^n \sum_{i \geq 0} (-1)^i q^{\binom{i+1}{2} + (i+1)k},$$

which establishes (7) for $k \geq 0$. Accordingly, for negative k , (2) yields the equality

$$Gm_k(q) = Gp(q)(1 - q^{1-k}T_{1-k}(q)) = Gp(q) T_{-k}(q),$$

so that (7) still holds. ■

Some remarks about the T_k 's defined above: First, for *each* integer k , T_k is analytic in the disk $\{|q| < 1\}$. Moreover, it can be verified that T_k is not a theta function. Note that, for each $k \in \mathbb{Z}$,

$$\sum_{n=-\infty}^{\infty} (-1)^n q^{\binom{n+1}{2} + nk} = 0$$

(turn n into $-n - 2k - 1$). Besides, the identity $\binom{k+i+1}{2} = \binom{k+1}{2} + \binom{i+1}{2} + ki$ yields the expression

$$T_k(q) = \frac{(-1)^k}{q^{\binom{k+1}{2}}} \sum_{n \geq k} (-1)^n q^{\binom{n+1}{2}}.$$

A further property of the T_k 's is given in (13) below.

We finally turn to the enumeration of the microstates which exhibit one electron at level k and zero electron at level k' . The number of all such microstates after the energy has been increased by n units is denoted by $m(n; k; k')$. Recall that $m(n, k)$ stands for the number of microstates with one electron at level k . Two basic formulas are

$$m(n; k; k') = m(n - (k - k'); k'; k), \quad (8)$$

$$m(n, k) - m(n; k; k') = m(n, k') - m(n; k'; k). \quad (9)$$

Move the electron from level k to level k' to obtain (8); the formal proof is straightforward. Besides, both expressions in (9) give the number of microstates which exhibit one electron at both levels k and k' conjointly.

COROLLARY 3. *Let $d = |k - k'|$; then*

$$\text{if } k' > k \quad \text{then } m(n; k; k') = \sum_{i \geq 0} m(n - id, k) - \sum_{i \geq 0} m(n - id, k'), \quad (10)$$

$$\text{if } k > k' \quad \text{then } m(n; k; k') = \sum_{i \geq 1} m(n - id, k') - \sum_{i \geq 1} m(n - id, k). \quad (11)$$

Proof. Note that all sums are finite. Identity (10) comes easily from (8) and (9), and identity (11) from (8) and (10). ■

4. IDENTITIES IN THE PHYSICAL MODEL

In this section, some of the results announced in [2] are demonstrated. The physical argument is only sketched, and the reader should refer to that paper for details.

In an isolated system (with evenly spaced energy levels and N electrons) with added energy $n \leq N$, the occupancy $\langle N_k \rangle$ of the k th energy level ($k \geq 1 - N$) is

$$\langle N_k \rangle = \frac{m(n, k)}{p(n)}.$$

In the so-called canonical ensemble, the system exchanges energy with a medium, so that n fluctuates. The probability of a microstate with added energy $n \leq N$ is proportional to $e^{-\beta n} p(n)$, where $e^{-\beta}$ is the Boltzmann factor (β is the temperature reciprocal). For the sake of averaging, N is assumed to be arbitrarily large, so that n may run through \mathbb{N} . Accordingly, the occupancy $\langle N_k \rangle_c$ of the k th energy level may be calculated as

$$\langle N_k \rangle_c = \frac{\sum_{n \geq 0} \langle N_k \rangle e^{-\beta n} p(n)}{\sum_{n \geq 0} e^{-\beta n} p(n)}.$$

According to Corollary 2, this formula may be written as

$$\langle N_k \rangle_c = e^{-\beta k^+} T_{|k|}(e^{-\beta}).$$

The average added energy $\langle n \rangle$ given by

$$\langle n \rangle = \frac{\sum_{n \geq 0} n e^{-\beta n} p(n)}{\sum_{n \geq 0} e^{-\beta n} p(n)} \quad (12)$$

may also be calculated from the $\langle N_k \rangle_c$'s as follows:

PROPOSITION 3.

$$\langle n \rangle = \sum_{k \geq 1} (2k - 1) \langle N_k \rangle_c$$

Proof. According to Corollary 1,

$$\begin{aligned}
 \langle n \rangle \sum_{n \geq 0} e^{-\beta n} p(n) &= \sum_{n \geq 0} n e^{-\beta n} p(n) \\
 &= \sum_{n \geq 0} \sum_{k \geq 1} (2k-1) m(n, k) e^{-\beta n} \\
 &= \sum_{k \geq 1} (2k-1) \sum_{n \geq 0} m(n, k) e^{-\beta n} \\
 &= \sum_{k \geq 1} (2k-1) \sum_{n \geq 0} \langle N_k \rangle p(n) e^{-\beta n},
 \end{aligned}$$

which completes the proof. ■

Incidentally, notice the following identity. Denoting by $\sigma_1(p)$ the sum of all divisors of p , expression (12) reads, with $q = e^{-\beta}$,

$$\langle n \rangle = \sum_{n \geq 1} \frac{n}{q^{-n} - 1} = \sum_{n \geq 1} \sum_{i \geq 1} n q^{in} = \sum_{p \geq 1} \sigma_1(p) q^p.$$

Therefore, Proposition 3 together with Corollary 2 yields

$$\sum_{k \geq 1} (2k-1) q^k T_k(q) = \sum_{n \geq 1} \sigma_1(n) q^n. \quad (13)$$

In the grand canonical ensemble, the system exchanges energy and electrons with a medium, so that both n and N fluctuate. The energy level are indexed as in Fig. 1, but now with respect to the average number \bar{N} of electrons. Denote by d the shift $N - \bar{N}$, and assume \bar{N} to be arbitrarily large, so that d may run through \mathbb{Z} . The probability of a microstate with number of electrons N and added energy n is proportional to $e^{-\beta(n + (1/2)d^2)} p(n)$, and the occupancy $\langle N_k \rangle_{\text{gc}}$ of the k th energy level may be calculated by averaging $\langle N_{k+d} \rangle_{\text{c}}$ in the following way:

$$\langle N_k \rangle_{\text{gc}} = \frac{\sum_{d=-\infty}^{\infty} \langle N_{k+d} \rangle_{\text{c}} e^{-(1/2)\beta d^2}}{\sum_{d=-\infty}^{\infty} e^{-(1/2)\beta d^2}},$$

If the energy levels are indexed with respect to the Fermi level ($\bar{N} - \frac{1}{2}$), the Fermi-Dirac formula predicts, for the κ th level ($\kappa = k - \frac{1}{2}$), an occupancy

$$\langle N_{\kappa} \rangle_{\text{FD}} = \frac{1}{e^{\beta \kappa} + 1}.$$

THEOREM 2. *The occupancy $\langle N_k \rangle_{\text{gc}}$ coincides with the corresponding value of the Fermi-Dirac distribution:*

$$\langle N_k \rangle_{\text{gc}} = \langle N_{k-(1/2)} \rangle_{\text{FD}}. \quad (14)$$

Proof.

$$\begin{aligned} \langle N_k \rangle_{\text{gc}} \sum_{d=-\infty}^{\infty} e^{-(1/2)\beta d^2} &= \sum_{d=-\infty}^{\infty} \sum_{i \geq 0} (-1)^i e^{-\beta((1/2)d^2 + \binom{i+1}{2} + (i+1)(k+d))} \\ &= \sum_{d=-\infty}^{\infty} \sum_{i \geq 0} (-1)^i e^{-(1/2)\beta((d+i+1)^2 + (i+1)(2k-1))} \\ &= \sum_{i \geq 0} (-1)^i e^{-\beta(i+1)(k-(1/2))} \sum_{d=-\infty}^{\infty} e^{-(1/2)\beta d^2}, \end{aligned}$$

which yields the asserted formula. ■

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