Illustration of the Fermi–Dirac statistics

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The distribution of electrons in small one-dimensional systems is obtained under the assumption of evenly spaced energy levels. The method consists of considering isolated systems and shifting electrons from their zero-temperature location. The distribution is then expressed in terms of the number of partitions of integers. When the system is in thermal contact with an electrical insulator, the electron distribution is obtained by averaging the previous result with the Boltzmann factor as a weight. Finally, when the system is in thermal *and* electrical contact with a large medium, the Fermi–Dirac distribution emerges through averaging over the number N of electrons. The statistics of light emitted or absorbed by the electron gas is obtained without quantization of the optical field. Our rigorous though elementary treatment helps clarify concepts employed in statistical mechanics. © *1999 American Association of Physics Teachers.*

I. INTRODUCTION

When students are introduced to the field of semiconductor physics, they are provided as one of their basic tools with the Fermi–Dirac (FD) statistics giving the probability p that some energy level be occupied by an electron. Since the number of electrons (in a single spin state) at some level can only be 0 or 1, the average number of electrons, called "occupancy," is equal to the probability p. In laser diodes, for example, application of the FD distribution to the conduction and valence bands of the semiconductor provides the total number of stored electrons as a function of the electrical voltage applied to the diode. Some integrals perhaps require intricate approximations, but no conceptual difficulty arises.

It is, on the other hand, not so easy to explain from first principles the origin of the FD distribution unless the students are willing to spend time studying books on statistical mechanics. To be sure, the derivation of the FD distribution given for example in Ref. 1 is formally simple, but the concepts employed there do not apply to the small isolated systems that one may encounter in modern electronics. The principles of statistical mechanics are presented in many books, e.g., Refs. 2–4. But most of them discuss the general properties of large systems on the basis of concepts that are difficult to comprehend in an intuitive manner. Many authors recognize that fact and find it advisable, from a pedagogical stand-point, to first treat small isolated systems.[5]

The present discussion relating to one-dimensional electronic systems has apparently not been given earlier in book form. Its goal is twofold. One is to provide exact expressions for electron occupancies in small systems. The other is to clarify concepts employed in statistical mechanics. In particular, it is emphasized that the temperature of small isolated systems is not a well-defined quantity. Accordingly, the word "temperature" will refer in this paper to the temperature of media of arbitrarily large size that may be in contact with the system considered. System temperatures are considered only in the so-called "thermodynamic" limit. The state of an isolated system is specified by the energy it contains. The state of a system in contact with a large medium may be specified by the *average* energy the system contains.

We first consider (possibly small) isolated systems. The simplicity of the method relies on the assumption that the energy levels are evenly spaced, with spacing ϵ. It is recalled in Sec. II that this is the case for one-dimensional harmonic oscillators. The assumption of evenly spaced levels may be a good approximation for realistic electronic devices.

Section III treats noninteracting electrons with either 0 or 1 electron allocated to the previously defined energy levels. The total energy is least when only levels below some particular level are occupied. Starting from that least-energy configuration, the total energy is incremented by $r\epsilon$ by submitting electrons to upward shifts summing up to the integer r, as illustrated in Fig. 1 for $r=6$. Electron states were obtained before in that manner in a very interesting paper by Schönhammer and Meden,[6] whose purposes, however, differ from ours. Exact analytical forms will be given for some of their numerical data.

Let us now give a preview of the results. For our model, the number $W(r)$ of ways the energy can be incremented by $r\epsilon$ is the number of *partitions* of r with, for example, $W(6)=11$. The letter "W" is employed here because this quantity is usually refered to as the "statistical weight" of the system. Each partition corresponds to an electronic configuration called a "microstate." Because all the microstates are equally likely to occur, according to the basic postulate of statistical mechanics, electron occupancies are obtained by dividing the number of electrons occupying some energy level (listed in Table I for $r=1-12$) by $W(r)$.

Fig. 1. System containing seven electrons. The energy levels are labeled by κ, with κ=0 at the Fermi level (defined one-half energy step above the zero-temperature highest energy). The column r=0 corresponds to zero temperature. The central part of the figure labeled r=6 exhibits the 11 ways (microstates) of incrementing the energy by E=6ε. The last column gives the number m_κ of electrons occupying some energy level, read off the central part. The average number of electrons $\langle N_\kappa \rangle$ is obtained by dividing m_κ by $W(6)=11$.

k	κ	r=0	r=6 (1 2 3 4 5 6 7 8 9 10 11)	m_κ
13	6.5			0
12	5.5			1
11	4.5			1
10	3.5			2
9	2.5			3
8	1.5			4
7	0.5			5
6	-0.5			6
5	-1.5			7
4	-2.5			8
3	-3.5			9
2	-4.5			10
1	-5.5			10
0	-6.5			11

Fig. 2. Ratio of the isolated electronic occupancy $\langle N_\kappa \rangle$ from Eq. (6) and the Fermi–Dirac (FD) occupancy $\langle N_\kappa \rangle_{FD}$ from Eq. (16) as a function of the FD occupancy, for the same (average) energy r taken as a parameter.

The analytic expression of the distribution in Eq. (6) forms the basis of most subsequent calculations. When the system considered is in contact with a heat bath ("canonical ensemble") the distribution is obtained by averaging the previous expression with the Boltzmann factor as a weight. This leads to the series in Eq. (9), Sec. IV. Finally, it is shown in Sec. V that when the system is in thermal *and* electrical contact with a large medium ("grand canonical ensemble") the FD distribution is recovered by further averaging. As indicated earlier and also recalled in Appendix A, the FD distribution may be obtained in a much more direct and general manner. Nevertheless, it is useful to outline the steps involved for a simple model.

Electron distributions and heat capacities for canonical and grand canonical ensembles at the *same well-defined temperature* are found to be significantly different, unless the system is large in a sense that will be made precise.

Electron distributions relating to isolated, canonical, and grand canonical ensembles, are compared in Table II for the case where the system (average) energy is equal to 6ε. When r is large (but not so large that the thermodynamic approximation is a valid one), even modern computers are unable to directly obtain electron occupancies. Our exact expressions are then required. Figure 2 shows that for (average) energies as high as 6000ε, isolated-system distributions differ from FD distributions. The agreement does not improve much by selecting temperatures in the FD distribution different from the one corresponding to the quoted energy.

One way of obtaining information about electron gases is to look at the emitted light. This is our motivation for discussing in Sec. VI the statistics of light in optical cavities containing electrons. It is proven in Appendix B that the Einstein prescription relating to emission and absorption by an atom agrees exactly with the statistical mechanical result.

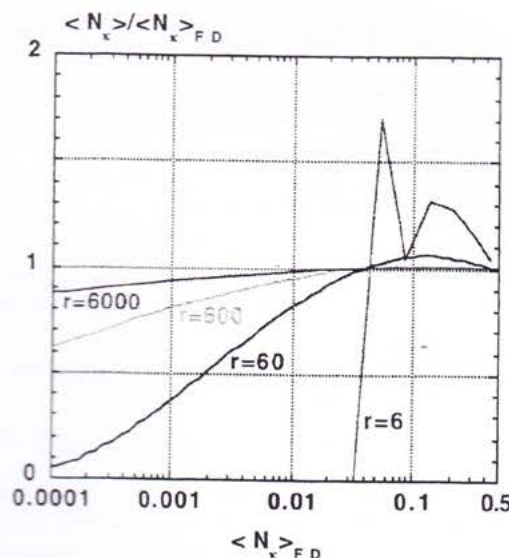The geometrical dimensions are considered constant throughout the paper and we are not interested in the pressure exerted by the electron gas on its boundaries. Thus subscripts introduced in thermodynamics to indicate that the volume is kept constant are omitted.

II. ONE-ELECTRON ENERGY LEVELS

The simplicity of the treatment given in the present paper rests on the assumption of evenly spaced energy levels. As is well known, this is the case for spinless particles forced to move in one-dimensional quadratic potentials (quantized harmonic oscillators). In the stationary state, the allowed energy levels are

$$\epsilon_k = (k + \tfrac{1}{2})\epsilon, \qquad (1)$$

where $k=0,1,...$ and ϵ is the energy spacing. If the factor 1/2 is suppressed by redefining the origin of the energy we have simply: $\epsilon_k = k\epsilon$. As a concrete example, consider electrons submitted to a very large magnetic field directed along the x axis and to an electrical potential $V(x)=x^2$. The magnetic field forces the electrons to one-dimensional motion and, furthermore, separates in energy electrons with spin 1/2 from those having spin −1/2, so that the two spin states may be treated separately. The electrical potential ensures harmonic motion.

Modern electronics employs quantum wires of small cross section (about 10 nm×10 nm) and length L (see Ref. 7 for a technical discussion). These wires are made up of small band-gap semiconductors embedded into higher band-gap media, so that the electrons get confined within the wire. If v denotes the electron (group) velocity in the energy range of interest, the spacing ϵ between adjacent energy levels is given by

$$\epsilon = \frac{hv}{2L}, \qquad (2)$$

where h denotes the Planck constant. A typical value of the energy spacing for L=1 μm is $\epsilon \approx 1$ meV. As pointed out in Ref. 6, in many cases the smooth variation of v may be neglected, in which case ϵ is approximately constant and our model is applicable. The fact that in most practical cases two spin states need to be considered may be handled as a rather straightforward generalization of the present treatment. Thus our model possesses some generality and may be applied to realistic systems.

III. MANY ELECTRONS

In the present section we consider an isolated system containing N electrons and total energy U. The electrons are supposed to be in the same spin state and their mutual direct interaction is neglected. Nevertheless, they influence each other because the Pauli principle forbids two electrons to be in the same state.

The column in Fig. 1 labeled r=0 represents electrons in their lowest energy states: $k=0,1,...,N-1$, the higher-lying states being empty, with N=7. For symmetry reasons to be explained later the states are labeled by $\kappa \equiv k-N+1/2$ instead of k. The system energy U_0 is obtained by adding up the energies of the N electrons. Since the energy spacing is ε,

$$U_0 = 0 + \epsilon + 2\epsilon + \cdots + (N-1)\epsilon = \frac{N(N-1)}{2}\epsilon. \qquad (3)$$

In the case of Fig. 1 with N=7 we have $U_0=21\epsilon$.

An important parameter is the energy $E \equiv r\epsilon$ (where r is an integer) added to the system on top of the zero-temperature energy U_0. This is realized by submitting electrons to upward shifts that sum up to the given energy increment. It is also required that the shifts be consistent with the Pauli exclusion principle. That is, two electrons should not end up at the same location. This condition is clearly fulfilled if the electron shifts are nonincreasing, beginning with the electron lying on top. Let us recall that electrons in the same spin state are *indistinguishable* particles. Accordingly, the exchange of two electrons would not result in a new configuration.

Observe further that, provided the energy added to the system is not too large (r<N), the lowest-lying electrons remain undisturbed. The number of electrons then becomes irrelevant, resulting in great simplification. If this is the case, the electron gas is said to be nearly degenerate. (Note that the word "degeneracy" here does not have the usual meaning that two or more states have the same energy.)

Each electron configuration corresponding to some energy increment E, or value of r, is called a microstate. The central part of Fig. 1 exhibits the W(6)=11 ways of incrementing the energy by E=6ε. Just looking at these microstates, the number m_k of electrons occupying some k level (for the whole set of microstates) is readily obtained. These numbers, listed on the right-hand side of Fig. 1, exhibit a symmetry with respect to a value of k located one-half energy step above the zero-temperature top electron energy. It is therefore advisable to label the states with a shifted value of k that we denote $\kappa \equiv k-\mu/\epsilon$ where $\mu=(N-1/2)\epsilon$. The symmetry relation then reads: $m_\kappa + m_{-\kappa} = W(r)$. Assuming that the microstates are equally likely, the occupancy $\langle N_k \rangle$ of level k is obtained by dividing m_k by the total number W(r) of microstates.

Some mathematical information concerning partitions is now given. As indicated earlier, a partition of r is a set of positive integers summing up to r. For example, 2,1,1 is a partition of 4 since 2+1+1=4. The numbers 2,1,1 are called "parts." Partitions of r up to 10 can be found in standard textbooks,[8] but a program was needed to generate partitions for larger values of r.

The *number* W(r) of partitions of r is available from MATHEMATICA. We have: W(0)=1 and, by convention, W(r)=0 if r<0. For most numerical calculations we found the approximation

$$W(r) \approx \frac{\exp(\pi\sqrt{2r/3})}{4r\sqrt{3}+3\sqrt{r}+2-(-1)^r} \qquad (4)$$

sufficiently accurate. The numerator of this expression alone suffices in the thermodynamic limit because we consider in that case only the logarithm S(r) of W(r), and extremely large values of r. The logarithm of the denominator $[\approx \ln(r)]$ of the expression in Eq. (4) is then negligible in comparison with the logarithm of the numerator ($\pi\sqrt{2r/3}$).

The generating function of W(r) reads[8,9]

$$\sum_{r=0,1,...} W(r)x^r = \prod_{n=1,2,...} (1-x^n)^{-1}. \qquad (5)$$

Notice that one may go from one microstate to another (called its conjugate) by exchanging electrons and holes (empty states) and reversing the energy scale. The conjugate pairs in Fig. 1, for example, are (1,11), (2,10), (3,9), (4,7), (5,8) while (6) is self conjugate.

Table I lists the values of m_κ for r=1−12. Only positive values of κ need be considered because of the symmetry of the distribution mentioned earlier. The occupancies $\langle N_\kappa \rangle \equiv m_\kappa / W(r)$ are given in the third column of Table II. The

Table I. Number $m_\kappa(r)$ of electrons at energy level κ.

κ	1	2	3	4	5	6	7	8	9	10	11	12
12.5	0	0	0	0	0	0	0	0	0	0	0	0
11.5	0	0	0	0	0	0	0	0	0	0	0	1
10.5	0	0	0	0	0	0	0	0	0	1	1	1
9.5	0	0	0	0	0	0	0	0	1	1	1	2
8.5	0	0	0	0	0	0	0	1	1	1	2	3
7.5	0	0	0	0	0	0	1	1	2	2	3	5
6.5	0	0	0	0	0	1	1	2	3	5	7	7
5.5	0	0	0	0	1	1	2	3	5	7	11	11
4.5	0	0	0	1	1	2	3	5	6	10	13	14
3.5	0	0	1	1	2	3	5	6	10	13	19	19
2.5	0	1	1	2	3	4	6	9	12	17	24	24
1.5	1	1	2	2	4	5	8	11	16	21	30	30
0.5	1	1	2	3	5	7	10	14	19	26	35	35
W(r)	1	2	3	5	7	11	15	22	30	42	56	77

Table II. Electron occupancies for r=6.

κ	m_κ	$\langle N_\kappa \rangle$	$\langle N_\kappa \rangle_c$	$\langle N_\kappa \rangle_{FD}$
6.5	0	0	0.032	0.032
5.5	1	0.091	0.052	0.053
4.5	1	0.091	0.084	0.087
3.5	2	0.182	0.131	0.138
2.5	3	0.273	0.202	0.213
1.5	4	0.364	0.300	0.313
0.5	5	0.455	0.430	0.435

significance of the last two columns of Table II will be discussed later.

The exact analytical expression of $m_\kappa(r)$, $\kappa > 0$, reads

$$m_\kappa(r) = - \sum_{i=1,2,...} (-1)^i W[r - i(\kappa + i/2)], \qquad (6)$$

the summation terminating when the argument of the W function (always an integer according to the definition of κ) is negative. The mathematical proof of Eq. (6), though simple in principle, is lengthy and will be given elsewhere.[10] For $r = 6$, Eq. (6) reads explicitly

$$m_\kappa(6) = W(5.5 - \kappa) - W(4 - 2\kappa) - W(1.5 - 3\kappa). \qquad (7)$$

For example, $m_{0.5}(6) = W(5) - W(3) + W(0) = 7 - 3 + 1 = 5$, in agreement with the number shown in Fig. 1 and in the tables.

From now on we take ϵ as the energy unit for the sake of brevity, that is, we set $\epsilon = 1$. In the typical case where $\epsilon = 1$ meV, this amounts to expressing energies in meV, a common practice in the field of solid-state physics. With that simplification we have $E \equiv r$. We also set the Boltzmann constant k_B equal to unity.

When r is extremely large the entropy $S(r) \equiv \ln[W(r)] \approx \pi\sqrt{2r/3}$. Within that approximation, the temperature is[1] $T(r) \equiv dr/dS \approx \sqrt{6r}/\pi$ and the electron contribution to the heat capacity reads

$$C(T) \equiv \frac{dr}{dT} = \frac{\pi^2}{3} T. \qquad (8)$$

This result shows how quickly one may recover the well-known fact that in the thermodynamic limit the electronic heat capacity is proportional to temperature. For most systems, however, ϵ is not truly a constant and Eq. (8) fails at high temperatures.

IV. CANONICAL ENSEMBLE

Suppose now that the electronic system is in thermal contact with an electrical insulator such as diamond, with temperature reciprocal β. The system energy E fluctuates. It is shown in Appendix A that electron occupancies are obtained in that situation by weighting the numbers $m_\kappa(r)$ given in Eq. (6) by the Boltzmann factor $\exp(-\beta r) = x^r$, where we have set $x \equiv e^{-\beta}$. The canonical occupancy thus reads (for $\kappa > 0$)

$$\langle N_\kappa \rangle_c = \frac{\sum_r m_\kappa(r) x^r}{\sum_r W(r) x^r} = - \sum_{i=1,2,...} (-1)^i x^{i(\kappa + i/2)}, \qquad (9)$$

where the sums over r run from 0 to infinity. The second expression in Eq. (9) has been obtained by inserting the expression of $m_\kappa(r)$ given in Eq. (6), and remembering that $W(r < 0) = 0$. Remarkably, the result no longer involves the partition of integers. For negative κ: $\langle N_\kappa \rangle_c = 1 - \langle N_{-\kappa} \rangle_c$.

An expression for $\langle N_\kappa \rangle_c$ derived by the method of second quantization was reported earlier in the appendix of Ref. 6. This alternative expression, which involves three recurrent infinite series, coincides with our expression in Eq. (9) to better than 16 decimal places, leaving little doubt that the two expressions are identical. A formal proof, however, has not been obtained.

With the help of Eq. (5) the normalization factor in Eq. (9), called the "statistical sum" or "partition function," may be written (the letter "Z" is from the german "Zustandsumme")

$$Z = \sum_r W(r) x^r = \prod_{n=1,2,...} (1 - x^n)^{-1}. \qquad (10)$$

Since the probability that energy r occurs is proportional to $W(r) x^r$, the average energy may be written

$$\langle r \rangle = \frac{\sum_r r W(r) x^r}{\sum_r W(r) x^r} = \frac{1}{Z} x \frac{dZ}{dx} = x \frac{d \ln(Z)}{dx}. \qquad (11)$$

Using the expression of Z in Eq. (10), the average system energy reads

$$\langle r \rangle = -x \frac{d}{dx} \sum_{n=1,2,...} \ln(1 - x^n) = \sum_{n=1,2,...} \frac{n}{x^{-n} - 1}. \qquad (12)$$

Alternatively, the average energy may be calculated by summing $2\kappa \langle N_\kappa \rangle_c$, where $\langle N_\kappa \rangle_c$ is given in Eq. (9), from $\kappa = 0.5$ to infinity. The resulting series seems to be different, but it can be shown to coincide with the result in Eq. (12). From Eq. (12) we calculate for example that $\langle r \rangle = 6$ when $\beta = 0.4851...$ (or $x \equiv e^{-\beta} = 0.6156...$). The canonical distribution in Eq. (9) is compared to the ($r = 6$) isolated system distribution in Table II for the value of β just quoted, that is, for an average energy equal to 6.

Since $\langle r \rangle$ is known explicitly as a function of β, it is easy to calculate the canonical heat capacity C (usually denoted C_V to emphasize that the volume is kept constant). Carrying out the differentiation and rearranging gives

$$C(T) = \frac{d\langle r \rangle}{dT} = \sum_{n=1,2,...} \left(\frac{n/2T}{\sinh(n/2T)} \right)^2. \qquad (13)$$

At high temperatures (thermodynamic limit) the sum in Eq. (12) may be replaced by an integral and we obtain

$$\langle r \rangle \approx \int_0^\infty dn \frac{n}{e^{n/T} - 1} = \frac{\pi^2}{6} T^2 - C(T) \approx \frac{\pi^2}{3} T. \qquad (14)$$

Within our model the approximate relation in Eq. (14) holds when T exceeds approximately 10 (i.e., $k_B T > 10\epsilon$). This result coincides with the one obtained before for isolated systems in the same limit.

V. GRAND CANONICAL ENSEMBLE

When the system is in thermal *and* electrical contact with a large medium, such as a piece of copper, the number of electrons in the system as well as the energy fluctuate. It is shown in Appendix A that the grand canonical distribution obtained by averaging the canonical distribution is indeed the FD distribution, namely

$$p \equiv \langle N_k \rangle_{FD} = \frac{1}{\exp[\beta(k - \mu)] + 1} \equiv \frac{1}{x^{\mu - k} + 1}, \quad x \equiv e^{-\beta}, \qquad (15)$$

where the Fermi level μ may be any real number.

The average number $\langle N \rangle$ of electrons, obtained by summing p over k from 0 to infinity, turns out to be equal to $\mu + 1/2$ when $\mu \gg 1$ (as implied by our near-degeneracy condition), irrespective of the value of β. From now on we require, for the sake of comparison with isolated systems and

canonical distributions, that $\langle N \rangle$ be an integer, that is, we assume that $\mu + 1/2$ is an integer. If the energy levels are labeled as in previous sections by $\kappa \equiv k - \mu$, the FD distribution reads

$$p = \frac{1}{x^{-\kappa} + 1}, \quad \kappa = ..., -1.5, -0.5, 0.5, 1.5, ... \qquad (16)$$

The average energy increment above the zero-temperature energy is, using the symmetry of the distribution,

$$\langle r \rangle_{FD} = 2 \sum_{\kappa = 0.5, 1.5, ...} \kappa p = \sum_{n=1,3,...} \frac{n}{x^{-n/2} + 1}. \qquad (17)$$

We find from this expression in Eq. (17) that the average energy $\langle r \rangle_{FD}$ is equal to 6 when $\beta = 0.5254...$ (or $x = 0.5913...$).

The FD distribution is shown in the last column in Table II for an average energy equal to 6 energy units. We observe that the canonical distribution differs appreciably from isolated system and Fermi–Dirac distributions. The differences between isolated and FD distributions are exemplified in Fig. 2, again for equal (average) energies, up to $\langle r \rangle \approx 6000$. Note the important discrepancies in the tails of the distributions. At electron occupancies of 10^{-4}, for example, the discrepancy exceeds 10% even when $\langle E \rangle$ is as large as 6000ϵ.

Let the heat capacity C_{FD} be defined as $d\langle r \rangle_{FD}/dT$. Using the expression in Eq. (17) for the average energy, we obtain after rearranging

$$C_{FD}(T) = 2 \sum_{n=1,3,...} \left(\frac{n/4T}{\cosh(n/4T)} \right)^2. \qquad (18)$$

The canonical heat capacity C differs from C_{FD} at low temperatures. For $T = 1$ (i.e., $T = 11$ K if $\epsilon = 1$ meV) for example, we calculate that $C = 0.84 C_{FD}$. The variations of C and C_{FD} as functions of T were illustrated before in Fig. 3 of Ref. 6.

VI. THERMAL LIGHT

One way of acquiring information about electron gases is to observe the emitted light. In the present section we consider a single-mode single-polarization optical cavity containing an electron gas. The light energy statistics follows from a concept implicit in the first (1900) Planck paper, which asserts that matter (electrons in the present case) may exchange energy with a wave at angular frequency ω only by units of $\hbar \omega$. Because the theory is semiclassical the word "photon," which strictly speaking has significance only when the light field is quantized, is avoided.

For our electron gas model with $\epsilon = 1$, resonant transitions may occur only when $\hbar \omega = q$, where q denotes some positive integer. Let an energy r^* be introduced in the optical cavity containing the nearly degenerate electron gas and initially no light. If the light energy is written as $m \hbar \omega = mq$, where m is a non-negative integer, the electron gas energy is $r = r^* - mq$ by conservation of energy. But, as we have seen, the number of ways this energy r may be realized is equal to the number $W(r)$ of partitions of r. Since, according to statistical mechanics, states of isolated systems corresponding to the same total energy are equally likely, the probability $P(m)$ of having light energy mq is

$$P(m) \propto W(r^* - mq), \qquad (19)$$

where the sign $\propto$ denotes proportionality. The actual probability is obtained by dividing $P(m)$ by its sum from $m = 0$ to $m = r^*/q$.

In order to measure $P(m)$ and verify the analytical result in Eq. (19), one should repeat a large number of times the following procedure: First, introduce in the cavity the energy r^* and wait long enough for a steady-state situation to establish itself. Then quickly replace the electrons by a detector that absorbs and measures the light energy mq left over in the cavity. In that way the statistics of m is being built up.

It is more usual to place the cavity in contact with a heat bath and perform measurements on the light steadily leaking out of the cavity. But in that case the system energy r^* fluctuates with a probability law given by the Boltzmann factor $\exp(-\beta r^*)$, where β denotes the heat-bath reciprocal temperature (see Appendix A). The light energy probability then reads using Eq. (19) (the subscript "c" is for "canonical")

$$P_c(m) \propto \sum_{r^* = mq \ldots \infty} P(m) \exp(-\beta r^*)$$

$$= \exp(-\beta mq) \sum_{r=0,1,...} W(r) \exp(-\beta r), \qquad (20)$$

where we have set again $r \equiv r^* - mq$.

The above expression is normalized by dividing it by its sum over m from 0 to ∞ (infinite geometric series). We then recover the usual expression for thermal light,[1]

$$P_c(m) = (1 - e^{-\beta q}) e^{-\beta mq}, \quad \beta \equiv 1/k_B T, \quad q \equiv \hbar \omega. \qquad (21)$$

Note that the above derivation relies only on the fact that $P(m)$ vanishes when the light energy mq exceeds the total available energy, a condition always fulfilled. In other words, the light leaking out of cavities is independent of the specific features of the model adopted in the description of matter (i.e., presently, of the electron gas).

Equation (19) may be obtained by an alternative method based on the Einstein concept of absorption and emission by individual atoms. Appendix B shows that the two methods agree with one another exactly (i.e., even for small systems).

VII. CONCLUSION

The assumption of equally spaced energy levels and near degeneracy affords great simplification in the statistical mechanical treatment of electron gases, all the quantities of interest being derived from the partition of integers. For small energies, the picture in Fig. 1 already provides a wealth of information. We find that the Fermi–Dirac distribution is not always a good approximation for small systems such as those employed in modern electronics, particularly at small occupancies. The exact electron distributions that we have obtained for isolated systems and for systems in thermal (but not electrical) contact with a large medium, should therefore prove useful.

When the system is in electrical and thermal contact with a large medium, all physical quantities, such as electron occupancies and heat capacities, are accurately predicted by the FD statistics even if the system is small, a well-known fact. It is also well-known that in the thermodynamic limit all three ensembles (isolated, canonical, and grand canonical) are equivalent. For our model, heat capacities are proportional to absolute temperature. This law fails at high tem-

peratures when it is not permissible to approximate the density of state near the Fermi level by a constant.

We have shown that the statistics of light intensity in optical cavities in equilibrium with the electron gas is given by the number of partitions of integers. This was done both by a direct calculation and by applying the Einstein concepts of atomic emission and absorption. The latter may be employed to generate sequences of emitted photons, thereby providing information on the noise properties of light-emitting diodes.

Though somewhat academic, the evenly spaced level model exhibits in a simple manner the virtues and limitations of the laws of statistical mechanics.

APPENDIX A: CANONICAL AND GRAND CANONICAL PROBABILITIES

Consider a possibly small system that may exchange heat with a large medium and let the number of states W_m of the medium be written as $\exp[S_m(U_m)]$ where U_m denotes the energy in the medium. The basic postulate of statistical mechanics is that the probability $p(U)$ of a system state with energy U is proportional to the number of medium states consistent with that value of U. The system and medium are supposed to interact weakly so that energies add up. Since $U \ll U_t$, where U_t denotes the total energy (medium+system), a first-order expansion of $S_m(U_m)$ $\equiv S_m(U_t - U)$ gives

$$p(U) \propto \exp(-\beta U), \quad \beta \equiv dS_m / dU_m. \quad (A1)$$

the derivative being evaluated at $U_m = U_t$. Remembering that, for the model treated in the main text, $U = U_0 + r$ where, according to Eq. (3), $U_0 = N(N-1)/2$ is a constant since N is a fixed integer, we have

$$p(U) \propto \exp(-\beta r) \equiv x^r, \quad x \equiv e^{-\beta}. \quad (A2)$$

The probability that some r value occurs is the product of the Boltzmann factor x^r and the number $W(r)$ of microstates (the "statistical weight" or "degeneracy factor") of the energy level r. Since the isolated system distribution in Eq. (6) $\langle N_\kappa \rangle \equiv m_\kappa(r)/W(r)$ depends on r, the canonical occupancy follows by averaging

$$\langle N_\kappa \rangle_c = \frac{\sum \langle N_\kappa \rangle W(r) x^r}{\sum W(r) x^r} = \frac{\sum m_\kappa(r) x^r}{\sum W(r) x^r}. \quad (A3)$$

where the sums run from $r = 0$ to infinity. This is the expression employed in Eq. (9).

Consider next a (possibly small) system that may exchange electrons and heat with a large medium and let the number of states W_m of the medium be written as $\exp[S_m(N_m, U_m)]$ where N_m and U_m denote, respectively, the number of electrons and energy in the medium. The probability $p(N, U)$ of a system state is proportional to the number of medium states consistent with these values. Since $N \ll N_t$ and $U \ll U_t$, where N_t and U_t denote, respectively, the total number of electrons and total energy (medium+system), a first-order expansion gives

$$p(N, U) \propto \exp(\alpha N - \beta U), \quad \alpha \equiv -\partial S_m / \partial N_m,$$
$$\beta \equiv \partial S_m / \partial U_m. \quad (A4)$$

Consider now a level k of the system, with energy ϵ_k. Let p_0 denote the probability that it is empty ($N = U = 0$) and p

the probability that it is occupied ($N = 1$, $U = \epsilon_k$). According to the expression of $p(N, U)$ in Eq. (A4) we have: $p/p_0 = \exp(\alpha - \beta\epsilon_k)$. Since $p_0 + p = 1$, the probability that the level k is occupied is

$$p = \frac{1}{\exp(\beta\epsilon_k - \alpha) + 1}. \quad (A5)$$

This is the celebrated Fermi–Dirac distribution. For our model with $\epsilon_k = k$, and setting $\alpha \equiv \beta\mu$, Eq. (A5) reads

$$p = \frac{1}{\exp(\beta k - \beta\mu) + 1} = \frac{1}{x^{k-\kappa} + 1} = \frac{1}{x^{-\kappa} + 1},$$
$$\kappa \equiv k - \mu. \quad (A6)$$

which is Eq. (16). In the nearly degenerate case the Fermi level μ is much larger than unity. We calculate from Eq. (A6) that $\langle N \rangle = \mu + 1/2$, and that the variance of N is equal to temperature T (in our reduced units). The distribution is symmetrical, as discussed in the main text, when $\mu + 1/2$ happens to be an integer.

Remembering that $U = r + N(N-1)/2$ according to Eq. (3), the probability law in Eq. (A4) factorizes into the Boltzmann factor considered before and a factor depending on N, namely

$$P(N) \propto \exp\left[\beta\left(\mu N - \frac{N(N-1)}{2}\right)\right]$$
$$\propto \exp\left[-\beta \frac{(N - \mu - 1/2)^2}{2}\right]. \quad (A7)$$

In going to the second expression a factor depending only on the constant α and β parameters has been dropped. It follows from the above expression of $P(N)$ that $\langle N \rangle = \mu + 1/2$ and that the variance of N is equal to temperature T if μ is large.

The canonical occupancy $\langle N_\kappa \rangle_c$ in Eq. (9) depends on $\kappa \equiv k - N + 1/2$. In the present situation N is not a fixed integer since it obeys the probability law in Eq. (A7). As N varies from one integral value to another, the canonical distribution gets shifted in energy up and down. The grand canonical occupancy is thus obtained by averaging $\langle N_{k-N+1/2} \rangle_c$ for some constant k value,

$$\langle N_k \rangle_{gc} = \frac{\sum \langle N_{k-N+1/2} \rangle_c P(N)}{\sum P(N)}, \quad (A8a)$$

where, according to Eq. (9),

$$2\langle N_\kappa \rangle_c = \left(1 + \frac{\kappa}{|\kappa|}\right) f(\kappa) + \left(1 - \frac{\kappa}{|\kappa|}\right)[1 - f(-\kappa)], \quad (A8b)$$

$$f(\kappa) \equiv -\sum_{i=1,2,\ldots} (-1)^i x^{i(\kappa + i/2)}. \quad (A8c)$$

It can be shown[10] that for $\mu \to \infty$ the expression in Eq. (A8) coincides with the Fermi–Dirac distribution in Eq. (A6) for any values of the parameters α and β (or μ and T).

APPENDIX B

In 1917 Einstein made a fundamental proposal relating to the behavior of atoms in optical cavities. For a single-mode cavity resonating at angular frequency ω and field energy $m\hbar\omega$, atoms in the lower state have a probability $m(t)dt$ (to

within a constant) of being promoted to the upper level during the time interval t to $t + dt$, the energy acquired by the atom being removed from the field. Atoms in the upper level have a probability $[m(t) + 1]dt$ of decaying to the lower level, giving up their energy to the field.

For N_l atoms in the lower level and N_u atoms in the upper level the transition probabilities thus read

$$P(m \to m - 1) = N_l(m, t)m,$$
$$P(m \to m + 1) = N_u(m, t)(m + 1). \quad (B1)$$

Obviously atomic populations depend on m. They may also depend explicitly on time, for example, because of random atomic motion. We assume that all the atomic states corresponding to some m value are being explored, so to speak, before the system jumps to some other m value, in which case $N_l(m, t)$ and $N_u(m, t)$ may be averaged over their explicit time dependence and denoted simply as $N_l(m)$ and $N_u(m)$.

Since the probabilities $P(m \to m \pm 1)$ no longer depend explicitly on time, Eq. (B1) describes a time-homogeneous birth–death (Markov) process whose theory is well established. The steady-state probability $P(m)$ obeys the detailed-balancing condition

$$P(m)P(m \to m - 1) = P(m - 1)P(m - 1 \to m). \quad (B2)$$

This relation is obvious for $m = 1$ because the probability is zero for negative m values, and the general expression follows by recurrence. A more formal proof can be found, for example, in Ref. 11.

If we introduce the expressions of the transition probabilities in Eq. (B1) into Eq. (B2), the m factor drops out, and we end up with

$$P(m)N_l(m) = P(m - 1)N_u(m - 1). \quad (B3)$$

Consider now specifically the electron gas treated in the main text, with unity spacing between adjacent levels, and set $\hbar\omega = q$, where q denotes any positive integer.

Let $n\uparrow(\kappa, q; r)$ denote the number of microstates of energy r having an electron at level κ and none at level $\kappa + q$, and $n\downarrow(\kappa, q; r)$ the number of microstates of energy r having an electron at level $\kappa + q$ and none at level κ. We have

$$n\uparrow(\kappa, q; r) = n\downarrow(\kappa, q; r + q). \quad (B4)$$

Indeed, the promotion of an electron of a microstate of energy r from κ to $\kappa + q$ is a microstate of energy $r + q$. This microstate may be converted back to the original microstate of energy r.

For simplicity, we now suppose that all κ values are equally likely (ignoring possible selection rules) and define $n\uparrow(q; r)$ and $n\downarrow(q; r)$ as the sums of $n\uparrow(\kappa, q; r)$ and $n\downarrow(\kappa, q; r)$, respectively, over all κ values. Values of $n\uparrow(q; r)$ and $n\downarrow(q; r)$ are illustrated in Table III (where the dots represent electrons) for $q = 1$ and $r = 0, 1, 2, \ldots$. Notice that the same values of $n\downarrow$ and $n\uparrow$ occur, shifted by one r unit and, incidentally, that $n\uparrow(1; r) - n\downarrow(1; r) = W(r)$.

Considering the interaction of light with electrons separated in energy by q, the averaged populations defined earlier read

$r =$	0	1	2	3	4	5	6
			↑				
		↑	↓	↑			
Fermi level -----	↑	↓					
			↑	↑	↓		
					↑		
$n\uparrow(1, r)$	1	2	4	7	12	19	30
$n\downarrow(1, r)$	0	1	2	4	7	12	19

$$N_l(m) = \frac{n\uparrow(q; r)}{W(r)}, \quad N_u(m) = \frac{n\downarrow(q; r)}{W(r)}, \quad (B5)$$

where $r = r^* - mq$, r^* being the given total energy (electrons+field). Introducing these definitions in the detailed balancing condition in Eq. (B3) we obtain

$$P(m) \frac{n\uparrow(q; r^* - mq)}{W(r^* - mq)}$$
$$= P(m - 1) \frac{n\downarrow(q; r^* - (m-1)q)}{W(r^* - (m-1)q)}. \quad (B6)$$

Because of the identity in Eq. (B4) (or rather its sum over κ) the numerators in Eq. (B6) cancel out, and we are left with

$$\frac{P(m)}{P(m-1)} = \frac{W(r^* - mq)}{W(r^* - (m-1)q)}. \quad (B7)$$

This is a recurrence relation whose solution is easily seen to coincide with Eq. (19). The Einstein method and statistical mechanics also agree if some k states are forbidden, as is the case for semiconductors.

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