Fluorescence from a few electrons

Jacques Arnaud
Mas Liron, F30440 Saint Martial, France

Laurent Chusseau
Centre d'Électronique et de Micro-optoélectronique de Montpellier, Université Montpellier II, F34095 Montpellier, France*

Fabrice Philippe[†]
Laboratoire d'Informatique, de Robotique et de Microélectronique de Montpellier, 161 rue Ada, F34392 Montpellier, France
(Received 5 June 2000)

Systems containing few fermions (e.g., electrons) are of great current interest. Fluorescence occurs when electrons drop from one level to another without changing spin. Only electron gases in a state of equilibrium are considered. When the system may exchange electrons with a large reservoir, the electron-gas fluorescence is easily obtained from the well-known Fermi-Dirac distribution. But this is not so when the number of electrons in the system is prevented from varying, as is the case for isolated systems and for systems that are in thermal contact with electrical insulators such as diamond. Our accurate expressions rest on the assumption that single-electron energy levels are evenly spaced, and that energy coupling and spin coupling between electrons are small. These assumptions are shown to be realistic for many systems. Fluorescence from short, nearly isolated, quantum wires is predicted to drop abruptly in the visible, a result not predicted by the Fermi-Dirac distribution. Our exact formulas are based on restricted and unrestricted partitions of integers. The method is considerably simpler than the ones proposed earlier, which are based on second quantization and contour integration.

I. INTRODUCTION

A number of remarkable experiments involving few electrons in semiconductors and free space, metal particles, and spin-1/2 atoms at low temperatures have been recently reported.[1,2] Only electrons are considered below. These collections of electrons may be isolated or in thermal contact with the environment, but, in any event, the number of particles is constant. The Fermi-Dirac (FD) distribution holds when electrons may be freely exchanged with a large reservoir (grand-canonical ensemble), but is inaccurate for the systems considered. The present paper provides simple and accurate formulas for electron occupancy and fluorescence for evenly spaced single-electron energy levels. Spontaneous emission is supposed to be weak enough not to perturb importantly the system state of equilibrium.[3] Only a vanishingly small Coulomb interaction between electrons[4] is considered. The time required for the system to reach equilibrium is not needed because averagings are performed over unlimited time scales. Quantum optics effects, such as resonance fluorescence or superradiance, will not be considered.

The assumption of evenly spaced single-electron energy levels is not as restrictive as one may think at first. Consider indeed one-dimensional devices such as the quantum wires employed in modern laser diodes.[1] If the wire is uniform over its length and the valence and conduction bands are parabolic in the energy-momentum space, the energy spacing ϵ between adjacent levels is not a constant. However, the variations of ϵ may be neglected near the Fermi level as long as the temperature is not too high. For zero-band-gap semiconductors such as $Pb_{0.84}Sn_{0.16}Te$, the energy-momentum re-

lationship is linear rather than parabolic, and ϵ is exactly a constant. Level spacings in small irregular metal particles (with a size on the order of 10 nm) are nearly uniform as a consequence of the mechanism of level "repulsion." The probability that adjacent levels are separated by ϵ is, for the appropriate ensemble, of the form $\epsilon^4 \exp(-\epsilon^2)$, a sharply peaked function of ϵ.[4] As is well known, the Landau levels that describe electron motion in uniform magnetic fields[2] are evenly spaced. These levels are highly degenerate, but the coupling between degenerate states (expressing the drift of electrons through the magnetic field lines) may be neglected over some period of time. Likewise, two- or three-dimensional harmonic oscillators, modeling, for example, the confinement of electrons in traps, exhibit degenerate evenly spaced levels. Our approach may be generalized to degenerate levels. It is appropriate to mention also that the density of states of (two-dimensional) quantum wells with parabolic bands is a constant within a subband. This implies that the energy-level spacing is constant on the average, though not exactly.

The amount of light spontaneously emitted by electronic systems depends on the optical-mode density of state, which is different for free-space, low-dimensional structures, or photonic band-gap materials. It is not the purpose of the present paper to discuss such problems. Because all comparisons are made at the same optical wavelength, terms depending on wavelength only (essentially the optical-mode density of state) may be dropped. The quantity that we calculate is the probability that the system exhibits an electron at level k and a hole (no electron) at level k', with $k - k' = \hbar\omega/\epsilon \equiv d$, where $\hbar$ denotes the Planck constant divided by 2π and ω the angular optical frequency of observation. In pure semi-

conductors, electron-momentum conservation entails that transitions may occur only symmetrically with respect to the Fermi level, implying that $k=(1+d)/2$, $k'=(1-d)/2$, with odd d, if $k=0$ labels the zero-temperature top electron. We will particularly consider the case where this condition holds.

Let us recall that, in statistical mechanics, isolated systems are described by microcanonical ensembles, systems that may exchange energy but not particles with a reservoir are described by canonical ensembles and systems that may exchange both energy and particles with a reservoir are described by grand-canonical ensembles. The Fermi-Dirac distribution[5] is applicable to finite systems only in the latter case. That is, the FD distribution is invalid for isolated systems and for systems that are in contact with an electrical insulator such as diamond. In the present context, ''finite'' (or ''small'' or ''mesoscopic'') means that $k_B T$, where T denotes the absolute electron gas temperature, is not necessarily large compared with the adjacent-level energy spacings ϵ. In grand-canonical ensembles, the fluorescence is proportional to the *product* of the probabilities that the upper level is occupied and that the lower level is empty. In canonical ensembles, it turns out that fluorescence is proportional to the *difference* between lower and upper levels occupancies. This is apparently a new result.

Exact formulas for the level occupancy in finite single-spin systems with evenly spaced levels in contact with a heat bath have been reported before.[4,6–9] Our method[6] consists of first enumerating the microstates of isolated systems. Subsequent averaging provides expressions for the canonical occupancies. This method is considerably simpler than the second-quantization methods and integral-transformation formulas employed in Refs. 4 and 8. The present paper generalizes the results reported in Ref. 6 to account for the fact that some electrons may change spin in the course of time. Simple, exact formulas for fluorescence are obtained for isolated systems and canonical ensembles. For arbitrary level energies and the canonical ensemble, known recurrence formulas[10] are satisfied by our more special, but explicit, forms.

The FD distribution is derived in Sec. II to set up the notation and to recall why, in grand-canonical ensembles, spin is properly accounted for by a twofold degeneracy. This method of accounting for the electron spin, however, is invalid in microcanonical or canonical ensembles because unpaired electrons may be in either one of two distinguishable states. Finite systems that exchange energy but not particles with a reservoir are considered in Secs. III and IV. In Sec. III, the electron spin is supposed to be strictly preserved and, for simplicity, it is supposed that there are as many electrons with spin up as with spin down. Formulas valid for single-spin electrons need only be multiplied by factors of 2 in that situation. In Sec. IV, electrons are allowed to change spin in the course of time (but not during a spontaneous emission event). For the sake of clarity, only essential formulas relating to canonical ensembles are given in the main text, detailed derivations and intermediate results being relegated to Appendixes A and B.

The purpose of Appendix A is to explain why the total number W of microstates of isolated systems is related to the partitions of integers, for single-spin-state electrons. It is shown that the number $m(k)$ of microstates whose level k is

occupied is simply related to W. The number $m(k;k')$ of microstates whose level k is occupied and level k' is empty is shown to be simply related to $m(k)$, and thus to W. Averaging, with the Boltzmann factor as a weight, provides the corresponding formulas in the canonical ensemble. Appendix B explains how the possibility that electrons may change spin in the course of time is accounted for.

II. FERMI-DIRAC DISTRIBUTION

The probability p that a system in thermal *and* electrical contact with a large medium contains N^+ electrons with spin up, N^- electrons with spin down, and energy U is proportional to the corresponding number of medium states (subscripts m) conveniently written as $\exp[S_m(N_m^+, N_m^-, U_m)]$ with S_m the medium entropy. If the system-medium contact is very weak, energies as well as particle numbers add up. A first-order expansion of S_m with respect to its arguments then gives

$$p(N^+, N^-, U) = C \exp(-\alpha N^+ - \alpha N^- - \beta U), \quad (1)$$

where C denotes a constant and

$$\beta = \frac{\partial S_m}{\partial U_m},$$

$$\alpha \equiv -\beta\mu = \frac{\partial S_m}{\partial N_m^+} = \frac{\partial S_m}{\partial N_m^-}. \quad (2)$$

Here, $\beta \equiv 1/k_B T$, where T denotes the temperature and μ the Fermi level. A single μ value occurs because the medium behavior is the same for electrons of opposite spins.

It follows from Eq. (1) that the probabilities $p^{(0)}$ that a nondegenerate state of energy ϵ_k is unoccupied, $p^{(1)}$ that it is occupied by an electron of either spin, and $p^{(2)}$ that it is occupied by two electrons are, respectively,

$$p^{(0)} = C,$$

$$p^{(1)} = Cz,$$

$$p^{(2)} = Cz^2, \quad (3)$$

with $z \equiv \exp(-\alpha - \beta\epsilon_k)$. Normalization $(p^{(0)} + 2p^{(1)} + p^{(2)} = 1)$ gives $C = 1/(1+z)^2$. The occupancy (average number of electrons) $n_{FD} = 2p^{(1)} + 2p^{(2)}$ of level k is therefore

$$n_{FD}(q;k) = \frac{2}{z^{-1}+1} = \frac{2}{\exp[\beta(\epsilon_k - \mu)]+1} = \frac{2}{q^{1/2-k}+1}, \quad (4)$$

where $q \equiv \exp(-\beta)$ denotes the Boltzmann factor. In the last expression it is assumed that $\epsilon_k = k$, where k denotes any relative integer. The separation ϵ between adjacent-level energies is taken as the energy unit, with a typical value for 1-μm-long quantum wires of $\epsilon = 1$ meV. In the last expression in Eq. (4), $k=1$ labels the level just above the top electron at $T=0$ K, and we have set $\mu = \frac{1}{2}$. Note that for large k values, $n_{FD}(q;k) \approx 2q^{k-1/2}$.

The average system energy added on top of the $T=0$ K energy is obtained by summing up the occupancy over all levels, and subtracting a similar sum for the $T=0$ K distribution. The result is[6]

$$r_{FD}(q) = \sum_{j=1,3,\ldots} \frac{j}{q^{-j/2}+1}. \tag{5}$$

In grand-canonical ensembles, occupancies at different levels are independent. For a single-spin state, this means that the probability that level k is occupied and level k' is empty is the product of level k occupancy and $(1-\text{level } k'$ occupancy). When the two-spin states are considered, we obtain

$$L_{FD}(q;k,k') = 2\frac{n_{FD}(q,k)}{2}\left(1 - \frac{n_{FD}(q,k')}{2}\right). \tag{6}$$

Fluorescence may indeed occur for 8 out of the 16 possibilities of occupancy of levels k and k' (no electron, spin-up electron, spin-down electron, or two electrons for each of the two levels). Because occupancies are independent, the sum of the probabilities that fluorescence events occur is found to be given by Eq. (6).

If the electron-momentum conservation law is enforced, we have $k=(1+d)/2$, $k'=(1-d)/2$, and the FD fluorescence in Eq. (6) reads after rearranging

$$L_{FD}(q;d) = \frac{2}{(q^{-d/2}+1)^2}. \tag{7}$$

Thus, the fluorescence in the grand-canonical ensemble is given by a simple function of temperature T and angular optical frequency of observation, ω. We will see that the canonical ensemble fluorescence is given by a simple series.

III. FLUORESCENCE WITHOUT SPIN FLIP

For single-spin electrons, the occupancy in isolated systems is given by a simple formula reported in Ref. 6. The proof, omitted in Ref. 6, is given in Appendix A of the present paper [see Eq. (A12)]. If the energy added to the system is denoted by r, the number $W(r)$ of configurations of the system is equal here to the number $p(r)$ of *partitions* of r. Indeed, microstates may be obtained by shifting electrons upward from their $T=0$ K locations by nonincreasing steps that sum up to r. Let us recall that a partition of r is a nonincreasing sequence of positive integers summing up to r. For example, $(2,1,1)$ is a partition of 4. The number $p(4)$ of partitions of 4 equals 5. By convention, $p(0)=1$ and $p(r)=0$ if $r<0$.

To illustrate the difference existing between the exact result and the Fermi-Dirac distribution, let us note that, for any microstate, the energy separation between the top electron and the lowest hole cannot exceed $r\epsilon$, where ϵ denotes as before the adjacent-level energy spacing. Accordingly, the fluorescence drops abruptly at an angular optical frequency $\omega = r\epsilon/\hbar$. When $r \gg 1$, a system temperature T may be defined:[6] $k_B T \approx \epsilon\sqrt{6r}/\pi$. As an example, room-temperature isolated systems with $\epsilon = 1$ meV should not emit visible light according to the exact formula, while some faint light is
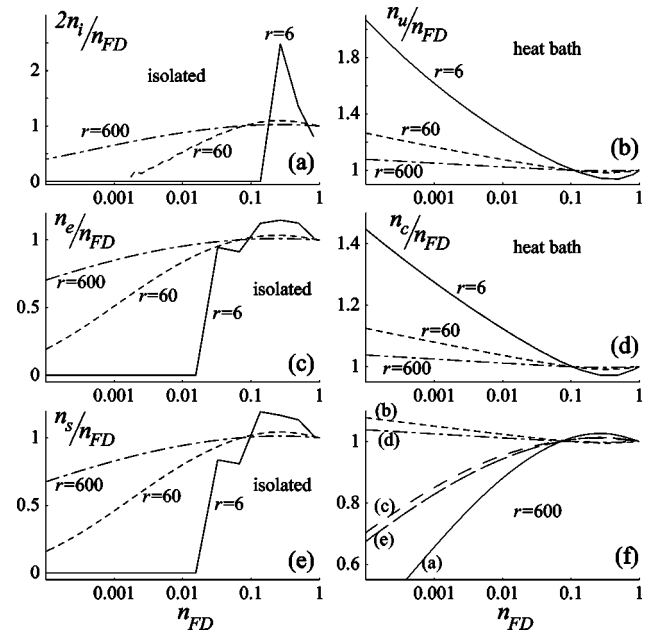

FIG. 1. Ratio of exact and Fermi-Dirac (n_{FD}) occupancies plotted as functions of n_{FD} at equal values of the average added energy r. The isolated single-spin-state electron occupancy in (a) was multiplied by 2 to account for the two-spin states. In (a) and (b) spin flip is not allowed. In (c) electrons of different spins may exchange energy but spin flip is not allowed. Cases (d) and (e) are the same as cases (b) and (c), respectively, except that spin flip is allowed. (f) collects previous results for an average added energy $r=600$.

expected according to the FD distribution.

In the present section, it is supposed that the electron spins are preserved in the course of time and that there are as many electrons with spin up and spin down, for simplicity. It then suffices to multiply the expressions for single-spin electron occupancy, average energy, and fluorescence, given in Appendix A, by factors of 2.

The occupancy reads, according to Eq. (A13),

$$n_u(q;k) = -2\sum_{j=1,2,\ldots}(-1)^j q^{jk+j(j-1)/2}. \tag{8}$$

Note that, for large k values, $n_u(q;k) \approx 2q^k$ so that $n_u(q;k)/n_{FD}(q;k) = \sqrt{q}$, if the expression for $n_{FD}(q;k)$ in Eq. (4) is used.

The average added energy reads[6]

$$r_u(q) = 2\sum_{j=1,2,\ldots}\frac{j}{q^{-j}-1}. \tag{9}$$

We first compare in Fig. 1(a) the occupancy in isolated systems with the FD occupancy. The former is obtained by multiplying $n_i(r;k)$ given in Eq. (A12) by a factor of 2 to account for the two-spin states. The FD occupancy is given in Eq. (4), with q expressed in terms of the average energy r with the help of Eq. (5). Note that, below 0.1, isolated-system occupancies are *smaller* than FD occupancies.

Consider next the case where the system is in contact with a heat bath. The ratio of the exact occupancy in Eq. (8) [where q is expressed in terms of the average energy r with the help of Eq. (9)] and the FD occupancy [Eqs. (4) and (5)]
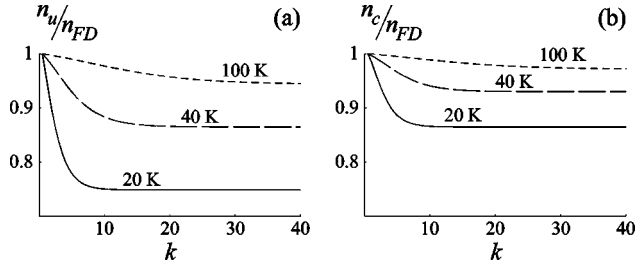
FIG. 2. This figure is similar to Fig. 1, but the comparison between canonical and grand-canonical ensembles is made at equal temperatures rather than at equal average energies. The energy-level spacing is supposed to be 1 meV, typical of 1-μm-long quantum wires. The parameter is the electron-gas absolute temperature T. (a) Spin flip is not allowed. (b) Spin flip is allowed.

FIG. 3. Ratio of spontaneously emitted light power (fluorescence) from 1-μm-long quantum wires in contact with diamond (canonical ensemble) and copper (grand-canonical ensemble), respectively, as a function of $d \equiv \hbar\omega/\epsilon$. The parameter is the electron-gas absolute temperature T. (a) Spin flip is not allowed. (b) Spin flip is allowed.

is represented in Fig. 1(b) as a function of the FD occupancy for various values of the average energy r (namely, $r=6$, 60, and 600). Below 0.1, the exact occupancy *exceeds* the FD occupancy. Figure 2(a) shows that, when the comparison is made at equal temperatures T (instead of equal average energies), the opposite occurs. In Fig. 2, we have chosen to represent the occupancy ratios as functions of the level number k (referred to the Fermi level) instead of the FD occupancy.

To evaluate fluorescence, we need to know the number $m(r;k;k')$ of microstates of added energy r having an electron at level k and none at level $k'=k-d$, where $d \equiv \hbar\omega/\epsilon$. Appendix A shows that this quantity is easily expressible in terms of the numbers $m(r;k)$ of microstates having an electron at level k (irrespectively of other state occupancies). Averaging the result over r with q^r as a weight to account for energy fluctuations in the presence of a heat bath, the fluorescence is found to be [see Eq. (A9)]

$$L_u(q;k,k') = \frac{n_u(q;k') - n_u(q;k)}{q^{-d} - 1},\qquad (10)$$

where $n_u(q;k)$ is given in Eq. (8).

If the law of electron-momentum conservation is enforced, the fluorescence reads

$$L_u(q;d) = L_u\left(q; \frac{1+d}{2}, \frac{1-d}{2}\right).\qquad (11)$$

Recall that $q \equiv \exp(-\epsilon/k_B T)$ (where ϵ is typically 1 meV and room temperature corresponds to $k_B T = 26$ meV) and $d \equiv \hbar\omega/\epsilon$. The fluorescence ratio $L_u(q;d)/L_{FD}(q;d)$ according to Eq. (7) and Eq. (11) is represented in Fig. 3(a) as a function of d for different temperatures. It is interesting that canonical and grand-canonical fluorescences almost coincide at small wavelengths even though the occupancies are quite different in that limit.

IV. FLUORESCENCE WITH SPIN FLIP

Electron spins are now allowed to vary in the course of time (but not during a fluorescence event). The numbers N^+ and N^- of electrons with spin up and spin down, respectively, may fluctuate, but their sum $N^+ + N^- \equiv N$ remains constant if the system is isolated or in contact with an elec-
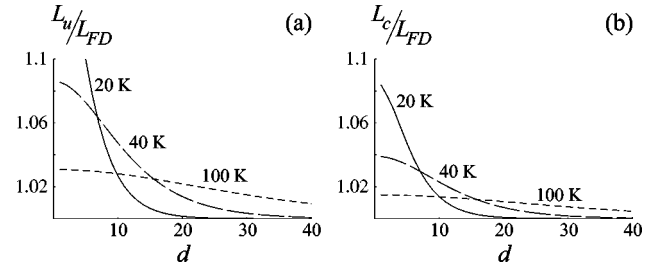
trically insulating heat sink such as diamond. The occupancy and fluorescence for coupled-spin electrons is derived from previous expressions through a succession of partitionings and averagings. Because the details are lengthy, they are relegated to Appendix B. Remarkably, many summations can be performed in closed form so that the final result is simple.

The occupancy reads

$$n_c(q;k) = \frac{\displaystyle\sum_{j=-\infty}^{+\infty} q^{j^2} n_u(q;k+j)}{\displaystyle\sum_{j=-\infty}^{+\infty} q^{j^2}},\qquad (12)$$

where $n_u(q;k)$ is given in Eq. (8). Comparisons with the FD distributions are exemplified in Figs. 1(d) and 2(b). With the help of theta functions[12] the average added energy may be written as a simple sum [see Eq. (B5)]

$$r_c(q) = 2 \sum_{j=1,2,\dots} \left(\frac{j}{q^{-j}-1} + \frac{(-1)^j j}{q^j - q^{-j}} \right).\qquad (13)$$

The fluorescence reads [see Eqs. (A14) and (B6)]

$$L_c(q;d) = \frac{\displaystyle\sum_{j=-\infty}^{+\infty} q^{j^2} L_u\left(q; j+\frac{1+d}{2}, j+\frac{1-d}{2}\right)}{\displaystyle\sum_{j=-\infty}^{+\infty} q^{j^2}},\qquad (14)$$

where $L_u(q;k,k')$ is given in Eq. (10). Fluorescence is illustrated in Fig. 3(b). Note that the exact result is closer to the FD result when electrons are allowed to change spin in the course of time.

V. CONCLUSION

When a (possibly small) system is in thermal and electrical contact with a large medium such as a piece of copper, the average number of electrons occupying some energy level (occupancy) is twice the value given by Fermi-Dirac formula. The fluorescence (light spontaneously emitted without electron-spin flip), defined in terms of the probability that an electron at level k may drop to level $k - \hbar\omega/\epsilon$ (ω denotes the angular optical frequency of observation), is also easily obtained. But when the system is isolated or in thermal con-

tact with an electrical insulator, electron occupancies are given by different expressions. Because modern electronics often employ short quantum wires supported by diamond heat sinks, it is important to have at our disposal precise expressions for occupancy and fluorescence in such situations. The expressions obtained in this paper were illustrated by comparison with the FD results. We considered the case where the electron spins are strictly maintained in the course of time (Sec. III) and the case where spin flip is allowed (Sec. IV). We found, for example, that small FD occupancies should be multiplied by approximately $\exp(-\epsilon/2k_BT) \approx 0.22$ if $\epsilon=1$ meV and $T=4$ K, a factor that differs significantly from unity. But, unexpectedly, the fluorescence turns out to be given rather accurately by the FD distribution.

Our mathematical approach is based on a direct enumeration of the microstates, and the results are expressed in terms of the number of partitions of integers. This method is considerably simpler than those previously reported for similar models, both conceptually and algebraically. A computer simulation has given results that are in very good agreement with the analytical formulas reported in this paper.

It is our intention to report in the future analytical and numerical results relating to mesoscopic laser-diode light fluctuations. A preliminary step consists of considering single-mode cavities incorporating the electron gas at thermal equilibrium, with one or two bands of states (for a single band, see Appendix A of the present paper). The intraband Auger effect and the stimulated transitions may be introduced at that stage. Next, the probability that low-lying electrons be promoted to high-lying levels by the action of a (quiet or fluctuating) pump and the probability that light quanta be absorbed are introduced. At low power, our simulation gives output light fluctuations that agree very well with elementary laser-noise theory predictions.[15] At high power, new effects (temperature fluctuations, spectral-hole burning, statistical fluctuations of the optical gain, etc.) occur that are difficult to handle analytically.[13] The analytical formulas reported in this paper are helpful to assess the accuracy of the simulation in special situations.

APPENDIX A: OCCUPANCY AND FLUORESCENCE FOR SINGLE-SPIN-STATE ELECTRONS: ARBITRARY ENERGY LEVELS

We are only concerned in the main text with evenly spaced one-electron energy levels $\{\epsilon_k\}$. Rigorous occupancy formulas are obtained in the present appendix by considering first arbitrary $\{\epsilon_k\}$. Eventually the number of levels is allowed to go to infinity.

Consider an isolated system whose nondegenerate one-electron level energies are, in increasing order, ϵ_1, ϵ_2, ..., ϵ_k, ..., ϵ_B, with $N \leq B$ single-spin electrons. According to the Pauli principle each level may be occupied by only 0 or 1 electron. The system energy U is therefore the sum of N of the ϵ_k. The purpose of this appendix is to evaluate the following.

(1) The number $W(N,U)$ of possible ways of obtaining some given U (number of microstates or ''statistical weight'').

(2) The number $m(N,U;k)$ of microstates whose level k

is occupied. The occupancy $n(N,U;k)$ of level k is defined as $m(N,U;k)/W(N,U)$.

(3) The number $m(N,U;k;k')$ of microstates whose level k is occupied and level k' is empty. The fluorescence $L(N,U;k;k')$ emitted by electrons dropping from level k to level k' is defined as $m(N,U;k;k')/W(N,U)$.

These evaluations will be presented in reversed order. Let us first relate the number $m(N,U;k;k')$ of microstates whose level k is occupied and level k' is empty to the numbers $m(N,U;k)$ defined above. For each microstate, let the electron at level k be transferred to the lower empty level k'. The number N of electrons is unaffected but the total energy gets reduced from U to $U-d$ where $d=\epsilon_k-\epsilon_{k'}>0$, and the roles of k and k' are reversed. The equality

$$m(N,U;k;k')=m(N,U-d;k';k) \tag{A1}$$

therefore holds. Now notice that

$$m(N,U;k)-m(N,U;k;k')=m(N,U;k')-m(N,U;k';k) \tag{A2}$$

because the two sides of the above equation count microstates whose levels k and k' are *both* occupied. When the expression in Eq. (A2) is introduced into Eq. (A1) iteration gives a recurrence relation for $m(N,U;k;k')$ that reads

$$m(N,U;k;k')=\sum_{j=1,2,\ldots} \times[m(N,U-jd;k')-m(N,U-jd;k)]. \tag{A3}$$

The above series terminates when the total energy vanishes, i.e., when jd exceeds U.

Consider next the $m(N,U;k)$ microstates whose levels k are occupied, and remove these electrons. The same number of microstates is obtained, with $N-1$ electrons, total energy $U-\epsilon_k$, and no electron at level k. The number of these new microstates may be written as the difference between the *total* number of microstates and the number of microstates whose level k is *occupied*. We have therefore the identity

$$m(N,U;k)=W(N-1,U-\epsilon_k)-m(N-1,U-\epsilon_k;k). \tag{A4}$$

After a sufficient number of iterations, either the energy or the number of electrons becomes negative and the last term vanishes. The quantity $m(N,U;k)$ may therefore be written as a finite sum

$$m(N,U;k)=-\sum_{j=1,2,\ldots}(-1)^j W(N-j,U-j\epsilon_k). \tag{A5}$$

The series terminates when j exceeds either N or U/ϵ_k.

We have the obvious identity (the number of occupied states for the whole set of microstates being written in two different manners)

$$NW(N,U)=\sum_{k\geq 1} m(N,U;k). \tag{A6}$$

A system in contact with a heat bath at temperature T is described by the canonical ensemble. Let us define as in the main text $q \equiv \exp(-\beta)$, where $\beta \equiv 1/k_B T$. The so-called partition function $Z(N,q)$ is the sum over U of $q^U W(N,U)$, and the average energy is $(q/Z)\partial Z(N,q)/\partial q$. When both sides of Eq. (A6) are multiplied by q^U and summed over U we obtain, using Eq. (A5),

$$Z(N,q) = \frac{1}{N} \sum_{k=1,2,\ldots} \sum_{U \geq 0} q^U m(N,U;k)$$

$$= -\frac{1}{N} \sum_{j=1,2,\ldots} (-1)^j \sum_{k=1,2,\ldots} q^{j\epsilon_k}$$

$$\times \sum_{U \geq 0} q^{U-j\epsilon_k} W(N-j, U-j\epsilon_k)$$

$$= -\frac{1}{N} \sum_{j=1,2,\ldots,N} (-1)^j Z(1,q^j) Z(N-j,q).$$

$$(A7)$$

Indeed, for a single electron ($N=1$), U may only take one of the ϵ_k values and the statistical weight W is unity. It follows that $Z(1,q)$ is the sum over k from 1 to B of q^{ϵ_k}. Note that $Z(0,q)=1$. Equation (A7) was obtained earlier[14] from a less direct proof.

The occupancy (average number of electrons) $n(q;k)$ of level k is equal to the sum over U of $q^U m(N,U;k)$, divided by $Z(N,q)$, where $m(N,U;k)$ is given in Eq. (A5) and $Z(N,q)$ is defined in Eq. (A7) from a recurrence relation. Thus

$$n(q;k) = \frac{-\sum_{j=1,2,\ldots} (-1)^j q^{j\epsilon_k} Z(N-j,q)}{Z(N,q)}. \quad (A8)$$

Expression (A8) was reported before.[10]

The probability that level k be occupied and that level k' be empty at temperature T is similarly obtained by summing $q^U m(N,U;k;k')$ over U, and dividing the result by $Z(N,q)$, where $m(N,U;k;k')$ is given in Eq. (A3). The result of the summation may be expressed as the *difference* of the lower and upper occupancies, according to

$$L(q;k,k') = \frac{n(q;k') - n(q;k)}{q^{\epsilon_{k'} - \epsilon_k} - 1}, \quad (A9)$$

where the occupancy $n(q;k)$ is given in Eq. (A8). Thus the fluorescence is equal to the difference between the occupancies at k' and k multiplied by the Bose function.

Let us now specialize the above formulas for the case where $\epsilon_k = k$, $k=1,\ldots,B$. Considering the displacement of the N electrons from their least-energy locations ($k=1-N$) beginning to the one on top, we observe that $W(N,U)$ is the number $p(P;N,r)$ of partitions of the *added energy* $r \equiv U - N(N+1)/2$ into at most N parts, none of them exceeding $P \equiv B-N$. Note that the numbers $p(P;N,r)$ may be obtained from a recurrence relation,[11] $p(P;N,r) - p(P;N-1,r) = p(P-1;N,r-N)$. Let us now change slightly our nota-

tion, letting $k=0$ denote the top electron in the least-energy configuration, and let us employ the added energy r instead of the total energy U as an argument. Equation (A5) reads

$$m(N,r;k) = - \sum_{j=1,2,\ldots} (-1)^j$$

$$\times p(P+j; N-j, r-jk-j(j-1)/2).$$

$$(A10)$$

If r does not exceed N and P, it is intuitive that $p(P;N,r)=p(r)$, where $p(r)$ denotes the number of unrestricted partitions of r. Equation (A10) then simplifies to

$$m(r;k) = - \sum_{j=1,2,\ldots} (-1)^j p(r-jk-j(j-1)/2).$$

$$(A11)$$

This expression was reported (for the first time to our knowledge) in Ref. 6. If N and P are infinite ($\{\epsilon_k\} = \mathbb{Z}$), Eq. (A11) holds for any finite value of r and the corresponding single-spin-state occupancy of an isolated system is

$$n_i(r;k) = m(r;k)/p(r). \quad (A12)$$

Averaging the numerator and denominator of above expression with q^r as a weight with r from 0 to ∞ gives the canonical occupancy[4]

$$n(q;k) = - \sum_{j=1,2,\ldots} (-1)^j q^{jk + j(j-1)/2}. \quad (A13)$$

Finally the expression in Eq. (A9) simplifies in the present situation to

$$L(q;k,k') = \frac{n(q;k') - n(q;k)}{q^{k'-k} - 1}. \quad (A14)$$

We have set up a Monte Carlo simulation program that enables us to recover previous analytical expressions. For the case of isolated systems, a constant probability per unit time is ascribed to level-changing events that preserve energy. The system eventually reaches a state of equilibrium with an electron distribution very close to the one derived from previous recurrence formulas. The Fermi-Dirac distribution is obtained in the limit of large B values, with temperatures and Fermi levels that depend on the energy given initially to the system. Our computer program may handle single-electron-level distributions that could be difficult to analyze theoretically (for example, two bands of states).

When the system is in thermal contact with a heat bat, electrons at level k are ascribed a probability per unit time, p, of being demoted to level $k-1$ and a probability $q p$ of being promoted to level $k+1$, provided these levels are empty. Strictly speaking, these prescriptions rest on an Einstein-type model of solids that supposes that the atoms are vibrating at frequency $\omega_{phonon} = \epsilon/\hbar$, where ϵ denotes as before the electronic level spacing. But the details of the thermalization model turn out to be rather unimportant. The computer program enabled us to reproduce the theoretical results with great accuracy. For example, when $B=100$, $\epsilon=1$ meV, and

$T = 100$ K, the numerical distribution fits the Fermi-Dirac distribution with a discrepancy not exceeding 0.2%.

When the electron gas is enclosed in a single-mode cavity, the probability that the cavity contains m light quanta is proportional to $W(r-md)$, where $W(r)$ denotes the statistical weight of the electron gas for an added energy r; see Appendix B of Ref. 6. If, initially, only the highest levels are occupied, we obtain exactly, from the recurrence relation satisfied by $p(P;N,r)$, variance(m)/average$(m) = (B+1)/6$.

APPENDIX B: OCCUPANCY AND FLUORESCENCE FOR TWO-SPIN-STATE ELECTRONS

In the present appendix we restrict ourselves to energy levels $\epsilon_k = k$, with $k = 1, 2, \ldots$, the origin of the energy being set at $k = 0$. Electrons are allowed to change spin in the course of time. We first consider an isolated system with constant numbers of spin-up and spin-down electrons (N^+ and N^-, respectively), electrons of different spins being allowed to exchange energy. Next, spin flip is allowed. Averaging, with the Boltzmann factor as a weight provides occupancies for the case where the systems are in contact with a heat bath. Occupancies in these various situations are illustrated in Fig. 1, again by comparison with the FD distribution.

Consider first an isolated system with N^+ spin-up electrons and N^- spin-down electrons, and suppose that the two subsystems may exchange energy but that spin flip is not allowed. Setting $N^+ + N^- \equiv 2N$ and $N^+ - N^- \equiv 2n$, the system least energy is

$$U_0 = \frac{N^+(N^++1)}{2} + \frac{N^-(N^-+1)}{2} = N(N+1) + n^2.$$
(B1)

If $r \geq n^2$ denotes the energy added to the system on top of $N(N+1)$, the remaining energy $s = r - n^2$ splits into r_1 in subsystem 1 and $r_2 = s - r_1$ in subsystem 2.

We have shown in Appendix A that, for the case presently considered and in the limit $N \to \infty$, the number of microstates for single-spin electrons is the number of partitions $p(r)$ of the excess energy r. The number of microstates relating to one particular splitting of s is therefore $p(r_1)p(r_2)$. Accordingly, occupancies are obtained by averaging single-spin-state occupancies shifted by $\pm n$, with a probability law proportional to $p(r_1)p(s-r_1)$ with r_1 running from 0 to s:

$n_e(r;k)$

$$= \frac{\displaystyle\sum_{r_1} [m(r_1;k-n)p(s-r_1) + m(s-r_1;k+n)p(r_1)]}{\displaystyle\sum_{r_1} p(s-r_1)p(r_1)},$$
(B2)

where $m(r;k)$ is given by Eq. (A11). Figure 1(c) compares $n_e(r;k)$ in Eq. (B2) to n_{FD} in Eqs. (4) and (5) for the case where $n = 0$ ($N^+ = N^-$ or $r = s$) and various values of the added energy.

When spin flip is allowed, $N^+ + N^- = 2N$ remains fixed, but $n \equiv (N^+ - N^-)/2$ may take any value that does not ex-

ceed $\sqrt{r}$, where r denotes as before the energy added on top of $N(N+1)$. If $r = 6$, for example, five values of n are permitted, namely, $n = 0$, $n = \pm 1$, and $n = \pm 2$. It thus suffices to sum the numerator and denominator of Eq. (B2) over permissible values of n. The occupancy reads

$n_s(r;k)$

$$= \frac{\displaystyle\sum_n \sum_{r_1} [m(r_1;k-n)p(s-r_1) + m(s-r_1;k+n)p(r_1)]}{\displaystyle\sum_n \sum_{r_1} p(s-r_1)p(r_1)},$$
(B3)

where the sum over r_1 is from 0 to $s = r - n^2$, and $m(r;k)$ is given Eq. (A11). The two terms in the numerator give equal contributions. Figure 1(e) compares $n_s(r;k)$ as given in Eq. (B3) with the FD distribution for various values of the added energy.

When the system is in contact with a heat bath at temperature reciprocal β, r fluctuates with a probability law q^r where, as before, $q \equiv \exp(-\beta)$. Accordingly, occupancies are obtained by multiplying the numerator and denominator of the previous expression in Eq. (B3) by q^r and summing over r from 0 to ∞. The denominator gives the sum over states

$$Z^*(q) = \sum_r q^r \sum_n \sum_{r_1} p(r_1)p(r-n^2-r_1)$$

$$= \left(\sum_r q^r p(r) \right)^2 \sum_n q^{n^2},$$
(B4)

which may be written as an infinite product.[12] The average added energy reads

$$r_c(q) = \frac{q}{Z^*} \frac{dZ^\star}{dq} = \sum_{j=1,2,\ldots} \left(\frac{2j}{q^{-j}-1} + \frac{(-1)^j 2j}{q^j - q^{-j}} \right).$$
(B5)

The expression for the occupancy may be reduced to a double sum, which coincides with the one given in Eq. (8), shifted by $\pm n$ and weighted by q^{n^2}. This final result is intuitive since unbalancing between N^+ and N^- increments the energy by n^2. We have

$$n_c(q;k) = \frac{\displaystyle\sum_n [n(q;k-n) + n(q;k+n)]q^{n^2}}{\displaystyle\sum_n q^{n^2}},$$
(B6)

where the sums over n run from $-\infty$ to $+\infty$, and $n(q;k)$ is given in Eq. (A13). The two terms in the numerator give the same contributions. The occupancy $n_c(q;k)$ may be expressed as a function of the average energy and k with the help of Eq. (B5). Comparison with the FD distribution is in Fig. 1(e).

Similarly the fluorescence is obtained by shifting k by n with a weight factor q^{n^2}.

*CEMII is Unité Mixte de Recherche n5507 associée au Centre National de la Recherche Scientifique.

†Also with Département de Mathématiques et Informatique Appliquées, Université Paul Valéry, F34199 Montpellier, France.

[1] *Quantum-Well Lasers*, edited by P. S. Zory (Academic Press, Boston, 1993). See Chap. 10.

[2] S. Pell and G. Gabrielse, Phys. Rev. Lett. **83**, 1287 (1999).

[3] B. Fain, Quantum Semiclassic. Opt. **8**, 755 (1996).

[4] R. Denton, B. Mühlschlegel, and D.J. Scalapino, Phys. Rev. B **7**, 3589 (1973).

[5] C. Kittel and H. Kroemer, *Thermal Physics* (Freeman, San Francisco, 1980).

[6] J. Arnaud, J.M. Boé, L. Chusseau, and F. Philippe, Am. J. Phys. **67**, 215 (1999).

[7] F. Philippe and J.M. Boé, J. Comb. Theory, Ser. A (to be published).

[8] K. Schönhammer and V. Meden, Am. J. Phys. **64**, 1168 (1996).

[9] F. Philippe, J. Phys. A **33**, L93 (2000).

[10] P. Borrmann, J. Harting, O. Mülken, and E.R. Hilf, Phys. Rev. A **60**, 1519 (1999). See Eq. (12).

[11] G.E. Andrew, in *Encyclopedia of Mathematics and Its Applications*, edited by G. C. Rota (Addison-Wesley, Reading, MA, 1976).

[12] B.C. Berndt, in *Theta Functions: From the classical to the modern*, edited by M. Ram Murty, CRM Proceedings and Lecture Notes (AMS, Providence, RI, 1993).

[13] J. Arnaud, Opt. Quantum Electron. **27**, 225 (1995).

[14] P. Borrmann and G. Franke, J. Chem. Phys. **98**, 2484 (1993).

[15] L. Chusseau and J. Arnaud (unpublished).