

Joule Expansion of a Pure Many-Body State

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We derive the Joule expansion of an isolated perfect gas from the principles of quantum mechanics. Contrary to most studies of irreversible processes which consider composite systems, the interesting and ignored degrees of freedom are here described by operators acting in the same many-body Hilbert space. Moreover, the expansion of the gas into the entire accessible volume is obtained for pure states. Still, the number particle density is characterized by a chemical potential and a temperature. We discuss the special case of a boson gas below the Bose condensation temperature.

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Irreversible processes can be described within the framework of quantum mechanics by taking into account a large amount of degrees of freedom. A small number of these degrees of freedom are involved in the considered process and the other ones are ignored. Most of the studies are concerned with composite systems consisting of a subsystem of interest coupled to one or several large reservoirs. For example, the decoherence and relaxation into thermal equilibrium of a quantum system is obtained by coupling it to a large heat bath [1]. In the context of transport, the quantum conductor under study is maintained out of equilibrium by connecting it to large free particle reservoirs [2]. The interesting physics occurs generally in the subsystem and the reservoirs' degrees of freedom are traced out [3]. The reservoirs are assumed large enough so that their states remain essentially unchanged during the studied process. It seems natural then to suppose that they are initially at thermal equilibrium.

It is often argued that the equilibrium states of the reservoirs result from their coupling to a thermal super-reservoir which is not taken into account explicitly in the model. Recently, it has been shown that such an *ad hoc* assumption is actually not necessary to understand the relaxation of a quantum system into thermal equilibrium [4–7]. It has been found that a boson bath initially in a *pure* state of macroscopically well-defined energy can induce this relaxation [7]. The thermalization process has thus been obtained as a consequence of the pure quantum-mechanical description of a truly isolated composite system. In this approach, the temperature of the asymptotic equilibrium state of the interesting subsystem is not introduced by hand by thermal averaging over the bath initial states. It is determined by the density of states of the bath and the macroscopic energy of its initial pure state.

In this Letter, we consider an isolated perfect quantum gas confined in a finite region of space. The gas particles do not interact with each other or with environmental degrees of freedom; they are only subject to a static confining potential. We show that the textbook example of an irreversible process, the Joule expansion, is a direct conse-

quence of the quantum mechanics principles. More precisely, we study the time evolution of the number particle density ensuing from an initial *pure* many-body state situated in a subregion of the total accessible volume. Following Refs. [5–7], we consider pure states of macroscopically well-defined energy. Contrary to the usually studied case of composite systems, the interesting and ignored degrees of freedom are here part of the same many-body system. However, we obtain, in the thermodynamic limit, a clear expansion of the gas into the entire accessible region for times much shorter than the Poincaré recurrence time of the system.

To simplify, we first restrict ourselves to the case of a one-dimensional perfect gas in an infinite square well potential of width L . The N indistinguishable particles, bosons or fermions, of mass m constituting the gas are described by the Hamiltonian

$$H_L = -\frac{1}{2m} \int_0^L dx \psi^\dagger(x) \partial_x^2 \psi = \sum_{k>0} \frac{k^2}{2m} c_k^\dagger c_k, \quad (1)$$

where $\psi^\dagger(x)$ and c_k^\dagger create, respectively, a particle at position x and in the single-particle eigenfunction $(2/L)^{1/2} \sin(kx)$. The sum runs over the wave vectors $k = n\pi/L$ where n is a positive integer. We use units in which $\hbar = k_B = 1$. In the following, we study the particle number density of the gas which can be written as

$$\rho(x, t) = \sum_k e^{ikx} \langle \hat{\rho}_k(t) \rangle, \quad (2)$$

where the sum runs over both positive and negative wave vectors k and $\langle \cdot \cdot \rangle$ denotes the average with respect to the initial gas state $|\psi\rangle$. The operators $\hat{\rho}_k$ are given by

$$\hat{\rho}_k(t) = \frac{1}{2L} \sum_{k' \neq 0, k} e^{ik(2k' - k)t/2m} \tilde{c}_k^\dagger \tilde{c}_{k' - k}, \quad (3)$$

where $\tilde{c}_k = \text{sgn}(k)c_{|k|}$. We remark that $\hat{\rho}_k^\dagger = \hat{\rho}_{-k} = \hat{\rho}_k$ and $\langle \hat{\rho}_0(t) \rangle = N/L$ for any state $|\psi\rangle$.

We assume that initially the N particles are confined in an interval $[0, \ell]$ where $\ell < L$, and that $|\psi\rangle$ is a state of macroscopically well-defined energy E . We are interested in the subsequent evolution of the density (2) in the thermodynamic limit $N \gg 1$ with finite mean distance ℓ/N and energy E/N . The initial gas state reads

$$|\psi\rangle = \sum_{|\alpha\rangle \in \mathcal{H}_E} \psi_\alpha |\alpha\rangle, \quad (4)$$

where $|\alpha\rangle$ refers to the N -particle eigenstates of the Hamiltonian H_ℓ given by (1) with the upper limit L replaced by ℓ . The wave vectors of the corresponding eigenmodes $(2/\ell)^{1/2} \sin(qx)$ are denoted by $q = n\pi/\ell$ where n is a positive integer. An eigenstate $|\alpha\rangle$ corresponds to a set of occupation numbers $\{n_q\}$ obeying $\sum_{q>0} n_q = N$. For fermions, n_q is restricted to the values 0 and 1. The Hilbert space \mathcal{H}_E is spanned by the states $|\alpha\rangle$ satisfying $E < \sum_{q>0} n_q q^2/2m < E + \delta E$ where δE is much smaller than E but much larger than the maximum level spacing of H_ℓ . In the thermodynamic limit, the dimension D of \mathcal{H}_E is practically proportional to δE and a density of states $n(E, N) = D/\delta E$ can be defined. Moreover, this density satisfies Boltzmann's relation

$$\ln[n(E, N)\delta E] \approx Ns\left(\frac{E}{N}, \frac{\ell}{N}\right), \quad (5)$$

where $s = S/N$ is the gas entropy per particle. As is well known, for a perfect gas, the relation (5) is a direct consequence of the exchange symmetry principle [8].

We now show that, in the thermodynamic limit, almost all normalized states (4) lead to the same particle number density. To obtain this result we use, following Refs. [5–7], the uniform measure on the unit sphere in \mathcal{H}_E

$$\mu(\{\psi_\alpha\}) = \frac{(D-1)!}{\pi^D} \delta\left(1 - \sum_{|\alpha\rangle \in \mathcal{H}_E} |\psi_\alpha|^2\right). \quad (6)$$

More precisely, we will evaluate the Hilbert space average and variance of $\langle \hat{\rho}_k(t) \rangle$ following from this normalized distribution. To do so, we note that, in the limit $N \gg 1$, the reduced distribution of a finite number q of components $\psi_{\alpha(1)}, \dots, \psi_{\alpha(q)}$ equals $\prod_{p=1}^q D \exp(-D|\psi_{\alpha(p)}|^2)/\pi$. With this Gaussian distribution, we obtain the Hilbert space average

$$\overline{\langle \hat{\rho}_k(t) \rangle} = \frac{e^{i\epsilon_k t}}{2LD} \sum_{\{n_q\} \in \mathcal{H}_E} \sum_{k'; q>0} e^{-ikk't/m} (q|k') (q|k' - k) n_q, \quad (7)$$

where $(q|k) = 2(L\ell)^{-1/2} \int_0^\ell dx \sin(qx) \sin(kx)$ and $\epsilon_k = k^2/2m$. This expression simply states that the Hilbert space average of the expectation value $\langle \hat{\rho}_k \rangle$ is equal to the microcanonical average at energy E of the operator $\hat{\rho}_k$. It can be further simplified using the following standard arguments [8]. The microcanonical probability distribution of the occupation number n_q is $P(n_q) = \hat{n}(E - n_q \epsilon_q, N -$

$n_q)/n(E, N)$ where $\epsilon_q = q^2/2m$ and \hat{n} is the density of states of the Hamiltonian $H_\ell - \epsilon_q c_q^\dagger c_q$. This density obeys Boltzmann's relation (5) with the corresponding entropy \hat{s} . Expanding this entropy in the energy $n_q \epsilon_q \ll E$ and number $n_q \ll N$ and taking into account that $\hat{s} = s$ in the thermodynamic limit result in $P(n_q) \propto \exp[-n_q(\epsilon_q - \mu)/T]$ where T and μ are given by

$$\frac{1}{T} = \partial_E S(E, N), \quad \frac{\mu}{T} = -\partial_N S(E, N). \quad (8)$$

Consequently, the microcanonical average numbers in (7) can be replaced by the Bose-Einstein or Fermi-Dirac occupation function at the microcanonical temperature T and chemical potential μ determined by the intensive parameters E/N and ℓ/N of the many-body state (4).

We define the Hilbert space variance σ^2 of $\langle \hat{\rho}_k \rangle$ as the average of $|\langle \hat{\rho}_k \rangle - \overline{\langle \hat{\rho}_k \rangle}|^2$ with respect to the measure (6). We find

$$\sigma^2 = \frac{1}{D^2} \sum_{|\alpha\rangle, |\beta\rangle \in \mathcal{H}_E} |\langle \alpha | \hat{\rho}_k(t) | \beta \rangle|^2 < \frac{1}{D} \langle \hat{\rho}_k(t)^2 \rangle_E, \quad (9)$$

where $\langle A \rangle_E = \sum_{|\alpha\rangle \in \mathcal{H}_E} \langle \alpha | A | \alpha \rangle / D$ denotes the microcanonical average at energy E of the observable A . The upper bound is simply obtained by replacing the sum over the states $|\beta\rangle \in \mathcal{H}_E$ by a sum over all the N -particle eigenstates $|\beta\rangle$ of the Hamiltonian H_ℓ . From the above arguments, one finds that the microcanonical distribution of two eigenmode occupation numbers is $P(n_q)P(n_{q'})$ with T and μ given by (8). As a consequence, the microcanonical average on the right-hand side of the inequality (9) is equal to a finite grand-canonical average and hence, as $D \sim \exp(N)$, the variance σ^2 vanishes exponentially in the thermodynamic limit. Therefore, for almost all states (4), the particle number density is given by (2) with the Fourier coefficients

$$\langle \hat{\rho}_k(t) \rangle = \frac{e^{i\epsilon_k t}}{2L} \sum_{k'; q>0} (q|k') (q|k' - k) f(q) e^{-ikk't/m}, \quad (10)$$

where $f(q) = [\exp(q^2/2mT - \mu/T) \mp 1]^{-1}$ depending on the bosonic or fermionic nature of the particles. To describe a gas state of macroscopic energy E , other choices than (4) are possible. For example, due to the exponential N dependence (5) of the density $n(E, N)$, one obtains the result (10) for almost all states of the Hilbert space spanned by the eigenstates $\{|n_q\rangle\}$ satisfying $\sum_q n_q = N$ and $\sum_q n_q \epsilon_q < E$. We also remark that the above derivation is not restricted to the observables $\hat{\rho}_k$. The result (10) can be generalized to any n -particle observables for $n \ll N$. The expression (10) holds for higher-dimensional systems, provided that the confining potential is independent of $x \in [0, L]$. More precisely, the number of particles $\rho(x)dx$ between x and $x + dx$ evolves according to (10) with f replaced by a sum over transverse eigenmodes. We con-

sider the case of macroscopic transverse dimensions towards the end of the Letter.

We now discuss the time evolution of the density ρ . For that purpose, it is useful, using the properties of the Dirac comb function [9], to rewrite (10) as

$$\begin{aligned} \langle \hat{\rho}_k(t) \rangle &= \frac{e^{i\epsilon_k t}}{4\pi L} \sum_{n,p} \int_{-\ell}^{\ell} dx \int_{-\ell}^{\ell} dx' \delta\left(x - x' + \frac{kt}{m} + 2nL\right) \\ &\quad \times e^{ikx} \sum_{\eta=\pm 1} \eta F(x - \eta x' + 2p\ell), \end{aligned} \quad (11)$$

where $F(x) = \int dq e^{iqx} f(q)$ is the Fourier transform of the grand-canonical occupation function f . The function F does not depend explicitly on the length ℓ , it depends only on the intensive parameters E/N and ℓ/N via the definitions (8). It assumes its maximum value $2\pi N/\ell$ at $x = 0$ and vanishes for large x . As an example, consider the classical Maxwell-Boltzmann limit, $\Lambda \ll \ell/N$ where $\Lambda = (\pi N/Em)^{1/2}$ is the de Broglie thermal wavelength ($E = NT/2$ here), where $F(x) \propto \exp(-\pi x^2/\Lambda^2)$. The expression (11) clearly shows that $\langle \hat{\rho}_k \rangle$ is periodic with period $t_k = 4Lm/k$ and $\langle \hat{\rho}_k(t_k/2) \rangle = \pm \langle \hat{\rho}_k(0) \rangle$ depending on the parity of kL/π . Consequently, the density ρ is periodic with period $4mL^2/\pi$ and $\rho(x, 2mL^2/\pi) = \rho(L - x, 0)$. Times of the order of mL^2 are practically inaccessible. For example, for He atoms and a length $L \simeq 10$ cm, the time period of the particle number density is of the order of a few days.

The gas expansion is described by the relaxation, for times $t \ll mL^2$, of the Fourier coefficients $\langle \hat{\rho}_k(t) \rangle$ corresponding to wavelengths of the order of the box length L . For these times and wavelengths, we obtain

$$\langle \hat{\rho}_k(t) \rangle \simeq \frac{\sin(k\ell)}{2\pi kL} F\left(\frac{kt}{m}\right), \quad (12)$$

up to a correction of order L^{-1} . The macroscopic wavelength components of the density ρ are of order unity at initial time and then relax according to (12). The gas evolution is hence essentially an expansion into the entire accessible volume, as illustrated by Fig. 1. This figure clearly shows that this evolution is very different from that of a single particle [10]. The results displayed in Figs. 1 and 2 are obtained by numerical evaluation of the sum (10). We remark that in the Maxwell-Boltzmann limit, the gas expansion described by (12) is characterized by an \hbar -independent time of the order of $L(m/k_B T)^{1/2}$ as expected from classical physics dimensional considerations. In the example already mentioned of He atoms in a box of 10 cm length, this time is of the order of 0.1 ms at $T = 300$ K and is thus far much shorter than mL^2 .

Interestingly, the macroscopic wavelength approximation (12) can be interpreted in quasiclassical terms as follows. The number particle density resulting from this approximation can be written as an integral over p of the distribution $w(x, p, t) = f(p) \sum_n \Pi_{\ell}(x - pt/m + 2nL)/2\pi$ where $\Pi_{\ell}(x) = 1$ for $|x| < \ell$ and 0 otherwise.

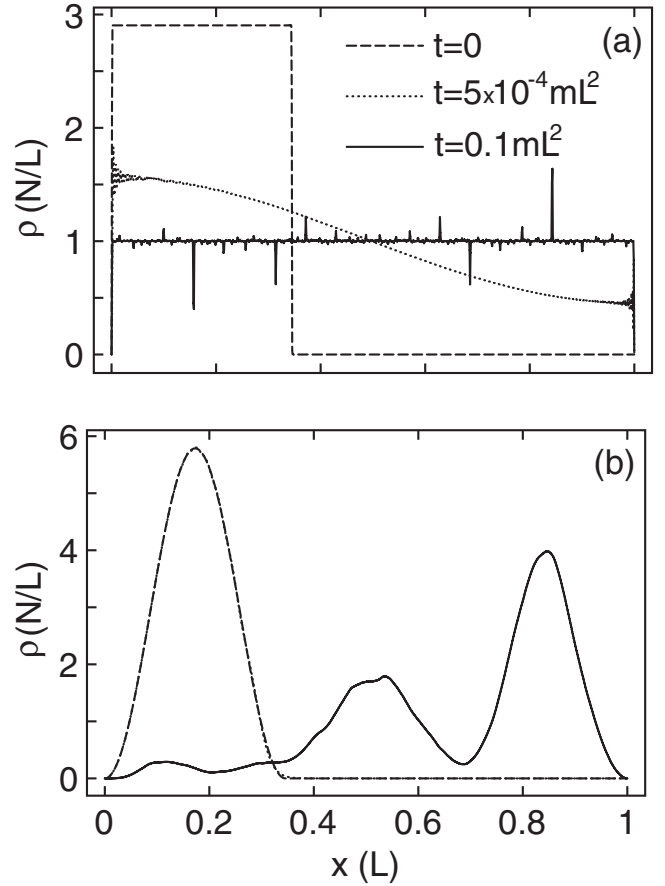


FIG. 1. Particle number density as a function of space for $\ell/L = 0.34567$ and times $t/mL^2 = 0, 5 \times 10^{-4}$, and 0.1 for (a) a 1D fermion gas at $T = 10^5/m\ell^2$ and $\exp(\mu/T) = 0.1$, (b) a 3D boson gas at $T = 0$ or, equivalently, a single particle initially in the ground state of the subbox $[0, \ell]$. In this last case, the first two curves cannot be distinguished.

This probability density describes classical particles which are initially distributed uniformly in the subbox $[0, \ell]$ with momenta p distributed according to the grand-canonical occupation function and which evolve freely between perfectly elastic collisions with the walls of the container $[0, L]$ [11]. The gas expansion given by (12) can be characterized by the time evolution of the particle current $J(t) = -\partial_t \int_0^\ell dx \rho(x, t)$. For short times, J is constant and equal to the Landauer current [12] $J_L = \int_{-\mu}^{\infty} d\epsilon / 2\pi [\exp(\epsilon/T) \mp 1]$ flowing through a perfect conductor from a reservoir at thermal equilibrium, the interval $[0, \ell]$, to an empty reservoir, the interval $[\ell, L]$; see Fig. 2. For longer times, the density ρ and hence the current J are well approximated by the longest wavelength terms of (2); see Figs. 1 and 2. Finally, the current J essentially vanishes. The long-time expansion is similar for periodic boundary conditions but with a symmetry plane at $\ell/2$.

Contrary to the quasiclassical approximation (12), the quantum number particle density determined by (10) does not relax into a steady state. As $\langle \hat{\rho}_k \rangle$ is time periodic with

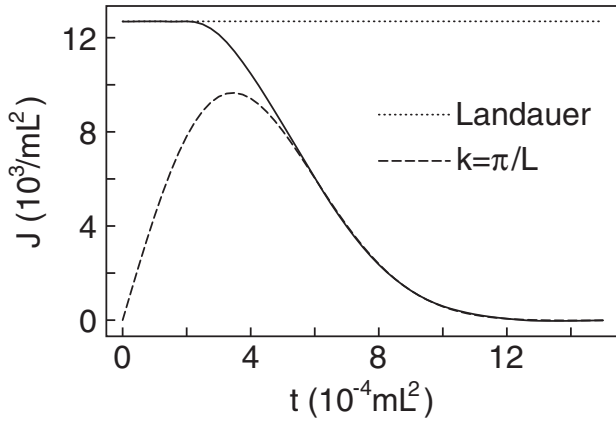


FIG. 2. Particle current J as a function of time for fermions, a fugacity of 0.1, $T = 10^5/m\ell^2$, and $\ell = 0.34567L$. The dotted line and dashed line are, respectively, the Landauer current and the contribution of the wave vector $k = \pi/L$.

period $t_k = 4Lm/k$, the density ρ fluctuates constantly, even in the Maxwell-Boltzmann limit. For the sake of clarity, we discuss this limit and a length $L > 2\ell$. From (11), we deduce that $|\langle \hat{\rho}_k(t) \rangle|$ is even and periodic with period $t_k/2$. Moreover, we find, for $0 < t < t_k/4$, $|\langle \hat{\rho}_k(t) \rangle| \simeq f(k/2)/4L$ for $t/t_k < \ell/2L$ and 0 elsewhere, provided that $t/t_k, |t/t_k - \ell/2L| \gg \Lambda/L$ where Λ is the de Broglie thermal wavelength. To show that the microscopic fluctuations of the density $\rho(x, t)$ do not disappear in the thermodynamic limit, we consider

$$M(t) = \int_0^L dx \left(\rho(x, t) - \frac{N}{L} \right)^2 = L \sum_{k \neq 0} |\langle \hat{\rho}_k(t) \rangle|^2, \quad (13)$$

which is a global measure of the difference between ρ and the uniform density N/L . The distance M decreases from the extensive value $M(0) \simeq (L/\ell - 1)N^2/L$ to finite values for $t \gg mL\Lambda$. For these times, all the Fourier components $|\langle \hat{\rho}_k \rangle|$ are of the order of L^{-1} , and M can be written as an integral over k on the intervals $[2m(pL - \ell)/t, 2m(pL + \ell)/t]$ where p is an integer. Consequently, the function $\rho(x, t) - N/L$ is nonvanishing in finite size regions, see Fig. 1, and changes with a characteristic time of the order of $mL\Lambda$.

We finally discuss the case of a gas in a tridimensional box of length L and rectangular cross-section $S \sim L^2$ initially confined in a subvolume $V = S\ell$ between $x = 0$ and $x = \ell$. The main difference with the unidimensional system is that here, for bosons, the average occupation number N_0 of the subbox V lowest eigenmode is macroscopic for E below the Bose condensation energy $E_B \propto N(N/V)^{2/3}/m$ [8]. We note that, in this case, the micro-canonical probability distribution of this occupation number is not of the grand-canonical form [13]. Whereas one eigenmode can be macroscopically populated here, the result $\rho = \bar{\rho}$ remains valid since the dimension D in (9) grows exponentially with N . For fermions and for bosons

with $E > E_B$, the gas expands according to (11) with F replaced by $F_{3D}(x) = S \int dq q \sin(qx) f(q)/2\pi x$. For bosons with $E < E_B$, the density $\rho = \rho_{\text{BEC}} + \rho_{\text{JE}}$ is the sum of two contributions corresponding, respectively, to the condensed and noncondensed bosons. The contribution ρ_{JE} is the zero chemical potential limit of the above case. The other contribution is very different since $\rho_{\text{BEC}}(x, t)$ equals N_0 times a single-particle position probability density; see Fig. 1. Therefore, though we consider pure states, the behavior of the boson gas is radically different below and above the Bose condensation temperature $T_B \propto E_B/N$.

In conclusion, we have obtained an irreversible evolution of physically relevant degrees of freedom of a many-body system without any coupling to environmental degrees of freedom. More precisely, we have shown that an isolated quantum perfect gas confined in a finite region of space tends to fill uniformly the total accessible volume, with the noticeable exception of the low energy 3D Bose gas. Moreover, whereas we consider pure gas states, the gas expansion is characterized by a chemical potential and a temperature and is well described by the Landauer formula for short times. It would be interesting to study the influence of interactions between the particles and with an environment. For a weak coupling to an environment, the behavior of the number particle density should be well described by our results for short enough times. The particle-particle interactions could induce a complete relaxation of the single-particle density matrix into a grand-canonical equilibrium state.

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