









Many particle systems

Many-particle systems often admit an (analytical) statistical description when their number becomes large.

In that sense they are simpler than few-particle systems. This feature has several diferent names – the law of large numbers, ergodicity, etc. – and it is one of the reasons for the spectacular successes of statistical physics.





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Phase space

The 3-dimensional physical space and 3-dimensional momentum space together constitute a 6-dimensional phase space, with coordinates {x, y, z, p_x , p_y , p_z }.

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Consider the 6-dimensional volume d^2V \equiv dV_x dV_p.
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In any Cartesian coordinate system, we can think of dV_x as a cube located at (x, y, z) with edge lengths dx, dy, dz, and similarly for dV_p . Then, as computed in this coordinate system, these volumes are

 $dV_x = dx \ dy \ dz, \ dV_p = dp_x \ dp_y \ dp_z,$

and

 $d^2V = dx dy dz dp_x dp_y dp_z$.









Momentum space and mass hyperboloid

The momentum-space diagram drawn in Fig. 3.2b has as its coordinate axes the components $(p^0, p^1 = p_1 \equiv p_x, p^2 = p_2 \equiv p_y, p^3 = p_3 \equiv p_z)$ of the 4-momentum as measured in some arbitrary inertial frame. Because the squared length of the 4-momentum is always $-m^2$,

$$\vec{p}\cdot\vec{p}=-(p^0)^2+(p_x)^2+(p_y)^2+(p_z)^2=-m^2, \eqno(3.4c)$$

the particle's 4-momentum (the tip of the 4-vector \vec{p}) is confined to a hyperboloid in momentum space. This *mass hyperboloid* requires no coordinates for its existence; it is the frame-independent set of points in momentum space for which $\vec{p} \cdot \vec{p} = -m^2$.

$$\mathcal{E} \equiv p^0 \tag{3.4d}$$

(with the \mathcal{E} in script font to distinguish it from the energy $E = \mathcal{E} - m$ with rest mass removed and its nonrelativistic limit $E = \frac{1}{2}mv^2$), and we embody the particle's spatial momentum in the 3-vector $\mathbf{p} = p_x \mathbf{e}_x + p_y \mathbf{e}_y + p_z \mathbf{e}_z$. Therefore, we rewrite the masshyperboloid relation (3.4c) as

$$\mathcal{E}^2 = m^2 + |\mathbf{p}|^2. \tag{3.4e}$$

If no forces act on the particle, then its momentum is conserved, and its location in momentum space remains fixed. A force (e.g., due to an electromagnetic field) pushes the particle's 4-momentum along some curve in momentum space that lies on the mass hyperboloid. If we parameterize that curve by the same parameter ζ as we use in spacetime, then the particle's trajectory in momentum space can be written abstractly as $\vec{p}(\zeta)$. Such a trajectory is shown in Fig. 3.2b.

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Volumes in phase space and distribution function

Now turn attention from an individual particle to a collection of a huge number of identical particles, each with the same rest mass m, and allow m to be finite or zero (it does not matter which). Examine those particles that pass close to a specific event \mathcal{P} (also denoted \vec{x}) in spacetime; and *examine them from the viewpoint of a specific observer, who lives in a specific inertial reference frame.* Figure 3.3a is a spacetime diagram drawn in that observer's frame. As seen in that frame, the event \mathcal{P} occurs at time t and spatial location (x, y, z).

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Specifically, the observer, in her inertial frame, chooses a tiny 3-volume

$$d\mathcal{V}_{\rm x} = dx \, dy \, dz \tag{3.5a}$$

centered on location ${\mathcal P}$ (little horizontal rectangle shown in Fig. 3.3a) and a tiny 3-volume

$$d\mathcal{V}_p = dp_x \, dp_y \, dp_z \tag{3.5b}$$

centered on **p** in momentum space (little rectangle in the p_x - p_y plane in Fig. 3.3b). Ask the observer to focus on the set S of particles that lie in dV_x and have spatial momenta in dV_p (Fig. 3.3). If there are dN particles in this set S, then the observer will identify

$$\mathcal{N} \equiv \frac{dN}{d\mathcal{V}_x d\mathcal{V}_p} \equiv \frac{dN}{d^2 \mathcal{V}} \tag{3.6}$$

as the number density of particles in phase space or *distribution function*.

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Turn now to the frame dependence of the particles' 3-volume $d\mathcal{V}_p$. As one sees from Fig. 3.3b, $d\mathcal{V}_p$ is the projection of the frame-independent mass-hyperboloid region $d\vec{\Sigma}_p$ onto the laboratory's *xyz* 3-space. Equivalently, it is the time component $d\Sigma_p^0$ of $d\vec{\Sigma}_p$. Now, the 4-vector $d\vec{\Sigma}_p$, like the 4-momentum \vec{p} , is orthogonal to the mass hyperboloid at the common point where they intersect it, and therefore $d\vec{\Sigma}_p$ is parallel to \vec{p} . This means that, when one goes from one reference frame to another, the time components of these two vectors will grow or shrink in the same manner; $d\vec{\Sigma}_p^0 = d\mathcal{V}_p$ is proportional to $p^0 = \mathcal{E}$, so their ratio must be frame independent:

$$\frac{d\mathcal{V}_p}{\mathcal{E}} = \text{(a frame-independent quantity)}.$$
(3.7b)

(If this sophisticated argument seems too slippery to you, then you can develop an alternative, more elementary proof using simpler 2-dimensional spacetime diagrams: Ex. 3.1.)

By taking the product of Eqs. (3.7a) and (3.7b) we see that for our chosen set of particles S,

 $d\mathcal{V}_x d\mathcal{V}_p = d^2 \mathcal{V} =$ (a frame-independent quantity); (3.7c)

and since the number of particles in the set, dN, is obviously frame-independent, we conclude that

$$\mathcal{N} = \frac{dN}{d\mathcal{V}_x d\mathcal{V}_p} \equiv \frac{dN}{d^2\mathcal{V}} = \text{(a frame-independent quantity)}.$$
(3.8)





Distribution function for photons

When dealing with photons or other zero-rest-mass particles, one often expresses \mathcal{N} in terms of the *specific intensity* I_v . This quantity is defined as follows (see Fig. 3.5). An observer places a CCD (or other measuring device) perpendicular to the photons' propagation direction **n**—perpendicular as measured in her reference frame. The region of the CCD that the photons hit has surface area dA as measured by her, and because the photons move at the speed of light c, the product of that surface area with c times the time dt that they take to all go through the CCD is equal to the volume they occupy at a specific moment of time:

$$d\mathcal{V}_x = dA \ cdt. \tag{3.11a}$$

Focus attention on a set S of photons in this volume that all have nearly the same frequency v and propagation direction **n** as measured by the observer. Their energies \mathcal{E} and momenta **p** are related to v and **n** by

$$\mathcal{E} = h\nu, \quad \mathbf{p} = (h\nu/c)\mathbf{n},$$
 (3.11b)

where *h* is Planck's constant. Their frequencies lie in a range dv centered on v, and they come from a small solid angle $d\Omega$ centered on $-\mathbf{n}$; the volume they occupy in momentum space is related to these quantities by

$$d\mathcal{V}_p = |\mathbf{p}|^2 d\Omega d|\mathbf{p}| = (h\nu/c)^2 d\Omega (hd\nu/c) = (h/c)^3 \nu^2 d\Omega d\nu.$$
(3.11c)

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FIGURE 3.5 Geometric construction used in defining the specific intensity I_{ν} .

The photons' specific intensity, as measured by the observer, is defined to be the total energy

$$d\mathcal{E} = h\nu dN \tag{3.11d}$$

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(where dN is the number of photons) that crosses the CCD per unit area dA, per unit time dt, per unit frequency dv, and per unit solid angle $d\Omega$ (i.e., per unit everything):

$$u_{\nu} \equiv \frac{d\mathcal{E}}{dAdtd\nu d\Omega}.$$
(3.12)

(This I_{ν} is sometimes denoted $I_{\nu\Omega}$.) From Eqs. (3.8), (3.11), and (3.12) we readily deduce the following relationship between this specific intensity and the distribution function:

$$\mathcal{N} = \frac{c^2}{h^4} \frac{I_\nu}{\nu^3}.$$
(3.13)

This relation shows that, with an appropriate renormalization, I_{ν}/ν^3 is the photons' distribution function.

Mean occupation number η

As an aid in defining the mean occupation number, we introduce the concept of the density of states: Consider a particle of mass m, described quantum mechanically. Suppose that the particle is known to be located in a volume $d\mathcal{V}_x$ (as observed in a specific inertial reference frame) and to have a spatial momentum in the region $d\mathcal{V}_p$ centered on p. Suppose, further, that the particle does not interact with any other particles or fields; for example, ignore Coulomb interactions. (In portions of Chaps. 4 and 5, we include interactions.) Then how many single-particle quantum mechanical states³ are available to the free particle? This question is answered most easily by constructing (in some arbitrary inertial frame) a complete set of wave functions for the particle's spatial degrees of freedom, with the wave functions (i) confined to be eigenfunctions of the momentum operator and (ii) confined to satisfy the standard periodic boundary conditions on the walls of a box with volume dV_x . For simplicity, let the box have edge length L along each of the three spatial axes of the Cartesian spatial coordinates, so $d\mathcal{V}_r = L^3$. (This L is arbitrary and will drop out of our analysis shortly.) Then a complete set of wave functions satisfying (i) and (ii) is the set $\{\psi_{j,k,l}\}$ with

$$\psi_{j,k,l}(x,y,z) = \frac{1}{L^{3/2}} e^{i(2\pi/L)(jx+ky+lz)} e^{-i\omega t}$$
(3.14a)

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The basis states (3.14a) are eigenfunctions of the momentum operator $(\hbar/i)\nabla$ with momentum eigenvalues

$$p_x = \frac{2\pi\hbar}{L}j$$
, $p_y = \frac{2\pi\hbar}{L}k$, $p_z = \frac{2\pi\hbar}{L}l$; (3.14b)

correspondingly, the wave function's frequency ω has the following values in Newtonian theory \aleph and relativity R:

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$$\hbar\omega = E = \frac{\mathbf{p}^2}{2m} = \frac{1}{2m} \left(\frac{2\pi\hbar}{L}\right)^2 (j^2 + k^2 + l^2);$$
 (3.14c)

R
$$\hbar\omega = \mathcal{E} = \sqrt{m^2 + \mathbf{p}^2} \rightarrow m + E$$
 in the Newtonian limit. (3.14d)

Equations (3.14b) tell us that the allowed values of the momentum are confined to lattice sites in 3-momentum space with one site in each cube of side $2\pi\hbar/L$. Correspondingly, the total number of states in the region $d\mathcal{V}_x d\mathcal{V}_p$ of phase space is the number of cubes of side $2\pi\hbar/L$ in the region $d\mathcal{V}_p$ of momentum space:

$$dN_{\text{states}} = \frac{dV_p}{(2\pi\hbar/L)^3} = \frac{L^3 dV_p}{(2\pi\hbar)^3} = \frac{dV_x dV_p}{\hbar^3}.$$
(3.15)

This is true no matter how relativistic or nonrelativistic the particle may be.

Thus far we have considered only the particle's spatial degrees of freedom. Particles can also have an internal degree of freedom called "spin." For a particle with spin s, the number of independent spin states is

$$g_s = \begin{cases} 2s+1 & \text{if } m \neq 0 \text{ (e.g., an electron, proton, or atomic nucleus)} \\ 2 & \text{if } m = 0 \text{ and } s > 0 \text{ [e.g., a photon } (s = 1) \text{ or graviton } (s = 2) \text{]} \end{cases}$$

1 if
$$m = 0$$
 and $s = 0$ (i.e., a hypothetical massless scalar particle)

(3.16)



Density of states & occupation number

$$\mathcal{N}_{\text{states}} \equiv \frac{dN_{\text{states}}}{d^2\mathcal{V}} = \frac{g_s}{h^3}$$

The ratio of the number density of particles to the number density of quantum states is obviously the number of particles in each state (the state's *occupation number*) averaged over many neighboring states—but few enough that the averaging region is small by macroscopic standards. In other words, this ratio is the quantum states' *mean occupation number* η :

$$\eta = \frac{\mathcal{N}}{\mathcal{N}_{\text{states}}} = \frac{h^3}{g_s} \mathcal{N}; \quad \text{i.e.,} \quad \boxed{\mathcal{N} = \mathcal{N}_{\text{states}} \eta = \frac{g_s}{h^3} \eta.}$$
(3.18)

The mean occupation number η plays an important role in quantum statistical mechanics, and its quantum roots have a profound impact on classical statistical physics.

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Classical or Boltzmann distribution function

The regime $\mu \ll -k_B T$, the mean occupation number is small compared to unity for all particle energies *E* (since *E* is never negative; i.e., *E* is never less than *m*). This is the domain of distinguishable, classical particles, and in it both the Fermi-Dirac and Bose-Einstein distributions become

$$\eta \simeq e^{-(E-\mu)/(k_BT)} = e^{-(\mathcal{E}-\tilde{\mu})/(k_BT)}$$

when $\mu \equiv \tilde{\mu} - m \ll -k_BT$ (classical particles).



Exercise 3.7 **Example: Observations of Cosmic Microwave Radiation (c) In actuality. Earth moves relative to the mean rest frame of the microwave backfrom Earth 🖪 💶 ground with a speed v of roughly 400 km s⁻¹ toward the Hydra-Centaurus region The universe is filled with cosmic microwave radiation left over from the big bang. At of the sky. An observer on Earth points his microwave receiver in a direction that each event in spacetime the microwave radiation has a mean rest frame. As seen in that makes an angle θ with the direction of that motion, as measured in Earth's frame. Show that the specific intensity of the radiation received is precisely Planckian in mean rest frame the radiation's distribution function η is almost precisely isotropic and thermal with zero chemical potential: form [Eqs. (3.23)], but with a direction-dependent Doppler-shifted temperature 1 $\eta = \frac{1}{e^{h\nu/(k_B T_o)} - 1}$, with $T_o = 2.725$ K. (3.29) $T = T_o\left(\frac{\sqrt{1-v^2}}{1-v\cos\theta}\right)$ (3.31)Here v is the frequency of a photon as measured in the mean rest frame. (a) Show that the specific intensity of the radiation as measured in its mean rest frame Note that this Doppler shift of T is precisely the same as the Doppler shift of the has the *Planck spectrum*, Eq. (3.23). Plot this specific intensity as a function of frequency of any specific photon [Eq. (2.33)]. Note also that the θ dependence frequency, and from your plot determine the frequency of the intensity peak. corresponds to an anisotropy of the microwave radiation as seen from Earth. (b) Show that η can be rewritten in the frame-independent form Show that because Earth's velocity is small compared to the speed of light, the anisotropy is very nearly dipolar in form. Measurements by the WMAP satellite give $T_o = 2.725$ K and (averaged over a year) an amplitude of 3.346×10^{-3} K for (3.30) $\eta = \frac{1}{e^{-\vec{p}\cdot\vec{u}_o/(k_B T_o)} - 1},$ where \vec{p} is the photon 4-momentum, and \vec{u}_o is the 4-velocity of the mean rest the dipolar temperature variations (Bennett et al., 2003). What, precisely, is the frame. [Hint: See Sec. 2.6 and especially Eq. (2.29).] value of Earth's year-averaged speed v?



Stress tensor (N) Notice that, if we multiply this S by the particles' mass m, the integral becomes the momentum density: $\mathbf{G} = m\mathbf{S} = \int \mathcal{N}\mathbf{p} \, d\mathcal{V}_p$ (3.32c) Finally, since the stress tensor **T** is the flux of momentum [Eq. (1.33)], its *j*-x component (*j* component of momentum crossing a unit area in the *y*-*z* plane per unit time) must be $T_{jx} = \int \frac{dN}{dydzdtd\mathcal{V}_p} p_j d\mathcal{V}_p = \int \frac{dN}{dxdydzd\mathcal{V}_p} \frac{dx}{dt} p_j d\mathcal{V}_p = \int \mathcal{N} p_j \frac{p_x}{m} d\mathcal{V}_p.$ This and the corresponding equations for T_{jy} and T_{jz} can be collected together into a single geometric, coordinate-independent integral: $T_{jk} = \int \mathcal{N} p_j p_k \frac{d\mathcal{V}_p}{m}, \quad \text{i.e.,} \quad \boxed{\mathbf{T} = \int \mathcal{N} \mathbf{p} \otimes \mathbf{p} \frac{d\mathcal{V}_p}{m}}.$ (3.32d) Notice that the number density *n* is the zeroth moment of the distribution function in momentum space [Eq. (3.32a)], and aside from factors 1/m, the particle flux vector is the first moment [Eq. (3.32b)], and the stress tensor is the second moment [Eq. (3.32d)]. All three moments are geometric, coordinate-independent quantities, and they are the simplest such quantities that one can construct by integrating the distribution function over momentum space. 46

Equations of state

If the Newtonian distribution function is isotropic in momentum space (i.e., is a function only of the magnitude $p \equiv |\mathbf{p}| = \sqrt{p_x^2 + p_y^2 + p_z^2}$ of the momentum, as is the case, e.g., when the particle distribution is thermalized), then the particle flux S vanishes (equal numbers of particles travel in all directions), and the stress tensor is isotropic: $\mathbf{T} = P\mathbf{g}$, or $T_{jk} = P\delta_{jk}$. Thus, it is the stress tensor of a perfect fluid. [Here *P* is the isotropic pressure, and **g** is the metric tensor of Euclidian 3-space, with Cartesian components equal to the Kronecker delta; Eq. (1.9f).] In this isotropic case, the pressure can be computed most easily as 1/3 the trace of the stress tensor (3.32d):

$$P = \frac{1}{3}T_{jj} = \frac{1}{3}\int \mathcal{N}(p_x^2 + p_y^2 + p_z^2)\frac{d\mathcal{V}_p}{m}$$
$$= \frac{1}{3}\int_0^\infty \mathcal{N} p^2 \frac{4\pi p^2 dp}{m} = \frac{4\pi}{3m}\int_0^\infty \mathcal{N} p^4 dp.$$
(3.37a)

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Here in the third step we have written the momentum-volume element in spherical polar coordinates as $dV_p = p^2 \sin \theta d\theta d\phi dp$ and have integrated over angles to get $4\pi p^2 dp$. Similarly, we can reexpress the number density of particles (3.32a) and the corresponding mass density as

$$n = 4\pi \int_0^\infty \mathcal{N} p^2 dp, \qquad \rho \equiv mn = 4\pi m \int_0^\infty \mathcal{N} p^2 dp. \qquad (3.37b)$$

Finally, because each particle carries an energy $E = p^2/(2m)$, the energy density in this isotropic case (which we shall denote by *U*) is 3/2 the pressure:

$$U = \int \frac{p^2}{2m} \mathcal{N} d\mathcal{V}_p = \frac{4\pi}{2m} \int_0^\infty \mathcal{N} p^4 dp = \frac{3}{2} P \qquad (3.37c)$$

[cf. Eq. (3.37a)].

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If we know the distribution function for an isotropic collection of particles, Eqs. (3.37) give us a straightforward way of computing the collection's number density of particles *n*, mass density $\rho = nm$, perfect-fluid energy density *U*, and perfect-fluid pressure *P* as measured in the particles' mean rest frame. For a thermalized gas, the distribution functions (3.22a), (3.22b), and (3.22d) [with $\mathcal{N} = (g_s/h^3)\eta$] depend on two parameters: the temperature *T* and chemical potential μ , so this calculation gives *n*, *U*, and *P* in terms of μ and *T*. One can then invert $n(\mu, T)$ to get $\mu(n, T)$ and insert the result into the expressions for *U* and *P* to obtain *equations of state* for thermalized, nonrelativistic particles:

$$U = U(\rho, T), \quad P = P(\rho, T).$$
 (3.38)

For a gas of nonrelativistic, classical particles, the distribution function is Boltzmann [Eq. (3.22d)], $\mathcal{N} = (g_s/h^3)e^{(\mu-E)/(k_BT)}$, with $E = p^2/(2m)$, and this procedure gives, quite easily (Ex. 3.8):

$n = \frac{g_s e^{\mu/(k_B T)}}{\lambda_{T dB}^3} = \frac{g_s}{h^3} (2\pi m k_B T)^{3/2} e^{\mu/(k_B T)},$	(3.39a)	
$U = \frac{3}{2}nk_BT, P = nk_BT.$	(3.39b)	
Notice that the mean energy per particle is (cf. Ex. 3.4b)		
$\bar{E} = \frac{3}{2} k_B T \; .$	(3.39c)	49



Relativistic Number-Flux 4-Vector **S** and Stress-Energy Tensor T

When we switch from Newtonian theory to special relativity's 4-dimensional spacetime viewpoint, we require that all physical quantities be described by geometric, frame-independent objects (scalars, vectors, tensors, . . .) in 4-dimensional spacetime. We can construct such objects as momentum-space integrals over the frame-independent, relativistic distribution function $\mathcal{N}(\mathcal{P}, \vec{p}) = (g_s/h^3)\eta$. The frame-independent quantities that can appear in these integrals are (i) \mathcal{N} itself, (ii) the particle 4-momentum \vec{p} , and (iii) the frame-independent integration element $d\mathcal{V}_p/\mathcal{E}$ [Eq. (3.7b)], which takes the form $dp_x dp_y dp_z/\sqrt{m^2 + \mathbf{p}^2}$ in any inertial reference frame. By analogy with the Newtonian regime, the most interesting such integrals are the lowest three moments of the distribution function:

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Meaning of the moments of ${\mathcal N}$

Zeroth

$$R = \int \frac{dN}{d\mathcal{V}_x d\mathcal{V}_p} \frac{1}{\mathcal{E}} d\mathcal{V}_p \tag{3.34}$$

(where of course $dV_x = dxdydz$ and $dV_p = dp_xdp_ydp_z$). This is the sum, over all particles in a unit 3-volume, of the inverse energy. Although it is intriguing that this quantity is a frame-independent scalar, it is not a quantity that appears in any important way in the laws of physics.

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Turn to the quantity T defined by the integral (3.33c). When we perform a 3+1 split of it in our chosen inertial frame, we find the following for its various parts:

$$T^{\mu 0} = \int \frac{dN}{d\mathcal{V}_x d\mathcal{V}_p} p^{\mu} p^0 \frac{d\mathcal{V}_p}{p^0} = \int \frac{dN}{d\mathcal{V}_x d\mathcal{V}_p} p^{\mu} d\mathcal{V}_p$$
(3.36a)

is the μ component of 4-momentum per unit volume (i.e., T^{00} is the energy density, and T^{j0} is the momentum density). Also,

$$T^{\mu x} = \int \frac{dN}{d\mathcal{V}_x d\mathcal{V}_p} p^{\mu} p^x \frac{d\mathcal{V}_p}{p^0} = \int \frac{dN}{dx dy dz d\mathcal{V}_p} \frac{dx}{dt} p^{\mu} d\mathcal{V}_p = \int \frac{dN}{dt dy dz d\mathcal{V}_p} p^{\mu} d\mathcal{V}_p$$
(3.36b)

is the amount of μ component of 4-momentum that crosses a unit area in the y-z plane per unit time (i.e., it is the x component of flux of μ component of 4-momentum). More specifically, T^{0x} is the x component of energy flux (which is the same as the momentum density T^{x0}), and T^{jx} is the x component of spatial-momentum flux—or, equivalently, the jx component of the stress tensor. These and the analogous expressions and interpretations of $T^{\mu y}$ and $T^{\mu z}$ can be summarized by

$$T^{00} = (\text{energy density}), \quad T^{j0} = (\text{momentum density}) = T^{0j} = (\text{energy flux}),$$

$$T^{jk} = (\text{stress tensor}).$$

(3.36c)

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Therefore [cf. Eq. (2.67f)], the τ of Eq. (3.33c) must be the stress-energy tensor introduced and studied in Sec. 2.13. Notice that in the Newtonian limit, where $\mathcal{E} \to m$, the coordinate-independent Eq. (3.33c) for the spatial part of the stress-energy tensor (the stress) becomes $\int \mathcal{N} \mathbf{p} \otimes \mathbf{p} \, d\mathcal{V}_p/m$, which is the same as our coordinate-independent Eq. (3.32d) for the stress tensor.





The solid right boundary is the point at which the electrons cease to behave like classical particles, because their mean occupation number η_e ceases to be $\ll 1$. As one can see from the Fermi-Dirac distribution (3.22a), for typical electrons (which have energies $E \sim k_B T$), the regime of classical behavior ($\eta_e \ll 1$; to the left of the solid line) is $\mu_e \ll -k_B T$ and the regime of strong quantum behavior ($\eta_e \simeq 1$; *electron degeneracy*; to the right of the solid line) is $\mu_e \gg +k_B T$. The slanted solid boundary in Fig. 3.7 is thus the location $\mu_e = 0$, which translates via Eq. (3.39a) to

$$\rho = \rho_{\text{deg}} \equiv 2m_p / \lambda_{\text{TdB}}^3 = (2m_p / h^3) (2\pi m_e k_B T)^{3/2} = 0.00808 (T/10^4 \text{ K})^{3/2} \text{ g cm}^{-3}.$$

Although the hydrogen gas is *degenerate* to the right of this boundary, we can still compute its equation of state using our kinetic-theory equations (3.37), so long as we use the quantum mechanically correct distribution function for the electrons—the Fermi-Dirac distribution (3.22a).⁹ In this electron-degenerate region, $\mu_e \gg k_B T$, the electron mean occupation number $\eta_e = 1/(e^{(E-\mu_e)/(k_BT)} + 1)$ has the form shown



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Zero T approximation

$$\eta_e = 1 \text{ for } p < p_F \equiv \sqrt{2m_e\mu_e}, \quad \eta_e = 0 \text{ for } p > p_F.$$
 (3.42)

(3.41)

Here p_F is called the *Fermi momentum*. (The word "degenerate" refers to the fact that almost all the quantum states are fully occupied or are empty; i.e., η_e is everywhere nearly 1 or 0.) By inserting this degenerate distribution function [or, more precisely, $\mathcal{N}_e = (2/h^3)\eta_e$] into Eqs. (3.37) and integrating, we obtain $n_e \propto p_F^3$ and $P_e \propto p_F^5$. By then setting $n_e = n_p = \rho/m_p$ and solving for $p_F \propto n_e^{1/3} \propto \rho^{1/3}$ and inserting into the expression for P_e and evaluating the constants, we obtain (Ex. 3.9) the following equation of state for the electron pressure:

$$P_e = \frac{1}{20} \left(\frac{3}{\pi}\right)^{2/3} \frac{m_e c^2}{\lambda_c^3} \left(\frac{\rho}{m_p / \lambda_c^3}\right)^{5/3}.$$
 (3.43)

Here

$$\lambda_c = h/(m_e c) = 2.426 \times 10^{-10} \,\mathrm{cm} \tag{3.44}$$

is the electron Compton wavelength.

The rapid growth $P_e \propto \rho^{5/3}$ of the electron pressure with increasing density is due to the degenerate electrons' being confined by the Pauli Exclusion Principle to regions of ever-shrinking size,

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Interior of white dwarfs

When the density of hydrogen in this degenerate regime is pushed on upward to

$$\rho_{\text{rel deg}} = \frac{8\pi m_p}{3\lambda_c^3} \simeq 9.8 \times 10^5 \,\text{g cm}^{-3} \tag{3.46}$$

(dotted vertical line in Fig. 3.7), the electrons' zero-point motions become relativistically fast (the electron chemical potential μ_e becomes of order m_ec^2 and the Fermi momentum p_F of order m_ec), so the nonrelativistic, Newtonian analysis fails, and the matter enters a domain of relativistic degeneracy (Sec. 3.5.4). Both domains, nonrelativistic degeneracy ($\mu_e \ll m_ec^2$) and relativistic degeneracy ($\mu_e \gtrsim m_ec^2$), occur for matter inside a massive white-dwarf star—the type of star that the Sun will become





Relativistic Density, Pressure, Energy Density, and Equation of State (isotropic systems)

 $\mathcal{E} = -\vec{u}_{rf} \cdot \vec{p}$ expressed in frame-independent form [Eq. (2.29)], $\mathcal{E} = p^0 = \sqrt{m^2 + p^2}$ in mean rest frame.

As in Newtonian theory, isotropy greatly simplifies the momentum-space integrals (3.33) that we use to compute macroscopic properties of the particles: (i) The integrands of the expressions $S^j = \int \mathcal{N} p^j (d\mathcal{V}_p/\mathcal{E})$ and $T^{j0} = T^{0j} = \int \mathcal{N} p^j p^0 (d\mathcal{V}_p/\mathcal{E})$ for the particle flux, energy flux, and momentum density are all odd in the momentum-space coordinate p^j and therefore give vanishing integrals: $S^j = T^{j0} = T^{0j} = 0$. (ii) The integral $T^{jk} = \int \mathcal{N} p^j p^k d\mathcal{V}_p/\mathcal{E}$ produces an isotropic stress tensor, $T^{jk} = Pg^{jk} = P\delta^{jk}$, whose pressure is most easily computed from its trace,

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Using these results and the relations $|\mathbf{p}| \equiv p$ for the magnitude of the momentum, $d\mathcal{V}_p = 4\pi p^2 dp$ for the momentum-space volume element, and $\mathcal{E} = p^0 = \sqrt{m^2 + p^2}$ for the particle energy, we can easily evaluate Eqs. (3.33) for the particle number density $n = S^0$, the total density of mass-energy T^{00} (which we denote ρ —the same notation as we use for mass density in Newtonian theory), and the pressure *P*. The results are

$$n \equiv S^{0} = \int \mathcal{N}d\mathcal{V}_{p} = 4\pi \int_{0}^{\infty} \mathcal{N}p^{2}dp,$$
$$\rho \equiv T^{00} = \int \mathcal{N}\mathcal{E}d\mathcal{V}_{p} = 4\pi \int_{0}^{\infty} \mathcal{N}\mathcal{E}p^{2}dp,$$
$$P = \frac{1}{3} \int \mathcal{N}p^{2}\frac{d\mathcal{V}_{p}}{\mathcal{E}} = \frac{4\pi}{3} \int_{0}^{\infty} \mathcal{N}\frac{p^{4}dp}{\sqrt{m^{2} + p^{2}}}$$

Equation of State for a Relativistic Degenerate Hydrogen Gas (zero T)

We can do so with the aid of the following approximation for the relativistic Fermi-Dirac mean occupation number $\eta_e = 1/[e^{(\mathcal{E}-\tilde{\mu}_e/(k_BT))} + 1]$:

$$\eta_e \simeq 1 \text{ for } \mathcal{E} < \tilde{\mu}_e \equiv \mathcal{E}_F; \text{ i.e., for } p < p_F = \sqrt{\mathcal{E}_F^2 - m^2},$$
 (3.50)

$$\eta_e \simeq 0 \text{ for } \mathcal{E} > \mathcal{E}_F; \text{ i.e., for } p > p_F.$$
 (3.51)

Here \mathcal{E}_F is called the relativistic *Fermi energy* and p_F the relativistic *Fermi momentum*. By inserting this η_e along with $\mathcal{N}_e = (2/h^3)\eta_e$ into the integrals (3.49) for the electron number density n_e , total density of mass-energy ρ_e , and pressure P_e , and performing the integrals (Ex. 3.10), we obtain results that are expressed most simply in terms of a parameter *t* (not to be confused with time) defined by

$$\mathcal{E}_F \equiv \tilde{\mu}_e \equiv m_e \cosh(t/4), \qquad p_F \equiv \sqrt{\mathcal{E}_F^2 - m_e^2} \equiv m_e \sinh(t/4).$$
 (3.52a)

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The results are

$$n_e = \frac{8\pi}{3\lambda_c^3} \left(\frac{p_F}{m_e}\right)^3 = \frac{8\pi}{3\lambda_c^3} \sinh^3(t/4), \qquad (3.52b)$$

$$o_e = \frac{8\pi m_e}{\lambda_c^3} \int_0^{p_F/m_e} x^2 \sqrt{1+x^2} \, dx = \frac{\pi m_e}{4\lambda_c^3} [\sinh(t) - t], \tag{3.52c}$$

$$P_e = \frac{8\pi m_e}{\lambda_c^3} \int_0^{p_F/m_e} \frac{x^4}{\sqrt{1+x^2}} \, dx = \frac{\pi m_e}{12\lambda_c^3} [\sinh(t) - 8\sinh(t/2) + 3t]. \quad (3.52d)$$

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White dwarfs

In a white-dwarf star, the protons, with their high rest mass, are nondegenerate, the total density of mass-energy is dominated by the proton rest-mass density, and since there is one proton for each electron in the hydrogen gas, that total is

$$\rho \simeq m_p n_e = \frac{8\pi m_p}{3\lambda_c^3} \sinh^3(t/4). \tag{3.53a}$$

By contrast (as in the nonrelativistic regime), the pressure is dominated by the electrons (because of their huge zero-point motions), not the protons; and so the total pressure is

$$P = P_e = \frac{\pi m_e}{12\lambda^3} [\sinh(t) - 8\sinh(t/2) + 3t].$$
 (3.53b)

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White DwarfImage: Straight of the straight of th

In the low-density limit, where $t \ll 1$ so $p_F \ll m_e = m_e c$, we can solve the relativistic equation (3.52b) for t as a function of $n_e = \rho/m_p$ and insert the result into the relativistic expression (3.53b); the result is the nonrelativistic equation of state (3.43). The dividing line $\rho = \rho_{\text{rel}} \deg = 8\pi m_p/(3\lambda_c^3) \simeq 1.0 \times 10^6 \text{ g cm}^{-3}$ [Eq. (3.46)] between nonrelativistic and relativistic degeneracy is the point where the electron Fermi momentum is equal to the electron rest mass [i.e., $\sinh(t/4) = 1$]. The equation of state (3.53a) and (3.53b) implies

 $P_e \propto \rho^{5/3}$ $\,$ in the nonrelativistic regime, $\rho \ll \rho_{\rm rel\,deg},$

 $P_e \propto
ho^{4/3}$ in the relativistic regime, $ho \gg
ho_{
m rel \, deg}.$

These asymptotic equations of state turn out to play a crucial role in the structure and stability of white dwarf stars (Secs. 13.3.2 and 26.3.5; Shapiro and Teukolsky, 1983;

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(3.53c)







Quantum gases: fermions and bosons (grand canonical ensemble)

The equation of state for a quantum ideal gas is

$$pV = kTln\Xi = \pm kT \sum_{j} ln[1 \pm e^{\beta\mu}e^{-\beta\varepsilon_j}]$$

The summation over states can be replaced by an integration over energy levels with:

$$\omega(\epsilon)d\epsilon = 2\pi \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} V \epsilon^{\frac{1}{2}} d\epsilon \qquad 3D$$

From this, derive the quantum virial expansion (where $\lambda = e^{\beta \mu}$):

$$\frac{\mathrm{P}}{\mathrm{k}\mathrm{T}} = \mp \frac{1}{\Lambda^3} \sum_{j=1}^{\infty} \frac{(\mp 1)^j \lambda^j}{j^{\frac{5}{2}}}$$
Equation of state of Bosons for any dimension ${\mathcal D}$

$$D(\epsilon) = \frac{V}{\Gamma(D/2)} \left(\frac{m}{2\pi\hbar^2}\right)^{D/2} \epsilon^{D/2-1}, \quad V = L^{D}.$$

Fundamental thermodynamic relations for BE gas: nV $\sum_{i=1}^{n} c_{i} c_{i} c_{i}^{\infty}$

$$\begin{split} & \frac{\mu_{p}}{k} = -\sum_{k} \ln\left(1 - ze^{-\beta \epsilon_{k}}\right) = -\int_{0}^{} d\epsilon \, D(\epsilon) \ln\left(1 - ze^{-\beta \epsilon}\right) = \frac{1}{\lambda_{T}^{D}} g_{D/2+1}(z) \\ & \mathcal{N} = \sum_{k} \frac{1}{z^{-1}e^{\beta \epsilon_{k}} - 1} = \int_{0}^{\infty} d\epsilon \, \frac{D(\epsilon)}{z^{-1}e^{\beta \epsilon_{k}} - 1} = \frac{V}{\lambda_{T}^{D}} g_{D/2}(z), \quad z < 1, \\ & U = \sum_{k} \frac{\epsilon_{k}}{z^{-1}e^{\beta \epsilon_{k}} - 1} = \int_{0}^{\infty} d\epsilon \, \frac{D(\epsilon)\epsilon}{z^{-1}e^{\beta \epsilon_{k}} - 1} = \frac{D}{2} k_{B}T \frac{V}{\lambda_{T}^{D}} g_{D/2+1}(z). \end{split}$$

V

The range of fugacity is limited to the interval $0 \le z \le 1$. At z = 1, the expression for N must, in some cases, be amended by an additive term to account for the possibility of a macroscopic population of the lowest energy level (at $\epsilon = 0$).



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Equations of state for Bosons and Fermions in 2 dimensions

- The classical limit is the straight line for positive *p* below the FD and above the BE equations.
- The effective repulsions in FD increase *p* while the effective attractions in BE decrease it, w. r. to the classical EoS.



Exercise 3.10 Derivation and Practice: Equation of State for Relativistic, Electron-Degenerate Hydrogen R 12

Derive the equations of state (3.52) for an electron-degenerate hydrogen gas. (Note: It might be easiest to compute the integrals with the help of symbolic manipulation software, such as Mathematica, Matlab, or Maple.)



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Transport coefficients



What are transport coefficients? An example is electrical conductivity κ_e . When an electric field E is imposed on a sample of matter, Ohm's law tells us that the matter responds by developing a current density

$\mathbf{j} = \kappa_e \mathbf{E}.$		

The electrical conductivity is high if electrons can move through the material with ease; it is low if electrons have difficulty moving. The impediment to electron motion is scattering off other particles—off ions, other electrons, phonons (sound waves), plasmons (plasma waves), . . . Ohm's law is valid when (as almost always) the electrons scatter many times, so they *diffuse* (random-walk their way) through the material. To compute the electrical conductivity, one must analyze, statistically, the effects of the many scatterings on the electrons' motions. The foundation for an accurate analysis is the Boltzmann transport equation (3.66).

(3.70a)

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Transport coefficients



Another example of a transport coefficient is thermal conductivity κ , which appears in the law of heat conduction

$$\mathbf{F} = -\kappa \boldsymbol{\nabla} T \,. \tag{3.70b}$$

Here F is the diffusive energy flux from regions of high temperature T to low. The impediment to heat flow is scattering of the conducting particles; and, correspondingly, the foundation for accurately computing κ is the Boltzmann transport equation.

Other examples of transport coefficients are (i) the coefficient of shear viscosity η_{shear} , which determines the stress T_{ij} (diffusive flux of momentum) that arises in a shearing fluid [Eq. (13.68)]

$$T_{ij} = -2\eta_{\text{shear}}\sigma_{ij}, \qquad (3.70c)$$

where σ_{ij} is the fluid's rate of shear (Ex. 3.19), and (ii) the diffusion coefficient *D*, which determines the diffusive flux of particles S from regions of high particle density *n* to low (Fick's law):

 $\mathbf{S} = -D\nabla n.$

(3.70d)

Transport coefficients

There is a *diffusion equation* associated with each of these transport coefficients. For example, the differential law of particle conservation $\partial n/\partial t + \nabla \cdot S = 0$ [Eq. (1.30)], when applied to material in which the particles scatter many times so $S = -D\nabla n$, gives the following diffusion equation for the particle number density:

$$\frac{\partial n}{\partial t} = D\nabla^2 n, \tag{3.71}$$

where we have assumed that D to this equation, we shall see the travel is proportional to the second characteristic of diffusive random Similarly, the law of energy $\mathbf{F} = -\kappa \nabla T$, leads to a diffusite thence for temperature [Ex. 3.1]

where we have assumed that *D* is spatially constant. In Ex. 3.17, by exploring solutions to this equation, we shall see that the root mean square (rms) distance \bar{l} the particles travel is proportional to the square root of their travel time, $\bar{l} = \sqrt{4Dt}$, a behavior characteristic of diffusive random walks.¹⁰ See Sec. 6.3 for deeper insights into this.

Similarly, the law of energy conservation, when applied to diffusive heat flow $\mathbf{F} = -\kappa \nabla T$, leads to a diffusion equation for the thermal energy density U and thence for temperature [Ex. 3.18 and Eq. (18.4)]. Maxwell's equations in a magnetized fluid, when combined with Ohm's law $\mathbf{j} = \kappa_e \mathbf{E}$, lead to diffusion equation (19.6) for magnetic field lines. And the law of angular momentum conservation, when applied to a shearing fluid with $T_{ij} = -2\eta_{\text{shear}}\sigma_{ij}$, leads to diffusion equation (14.6) for vorticity.

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Transport coefficients

These diffusion equations, and all other physical laws involving transport coefficients, are approximations to the real world-approximations that are valid if and only if (i) many particles are involved in the transport of the quantity of interest (e.g., charge, heat, momentum, particles) and (ii) on average each particle undergoes many scatterings in moving over the length scale of the macroscopic inhomogeneities that drive the transport. This second requirement can be expressed quantitatively in terms of the mean free path λ between scatterings (i.e., the mean distance a particle travels between scatterings, as measured in the mean rest frame of the matter) and the macroscopic inhomogeneity scale \mathcal{L} for the quantity that drives the transport (e.g., in heat transport that scale is $\mathcal{L} \sim T/|\nabla T|$; i.e., it is the scale on which the temperature changes by an amount of order itself). In terms of these quantities, the second criterion of validity is $\lambda \ll \mathcal{L}$. These two criteria (many particles and $\lambda \ll \mathcal{L}$) together are called diffusion criteria, since they guarantee that the quantity being transported (charge, heat, momentum, particles) will diffuse through the matter. If either of the two diffusion criteria fails, then the standard transport law (Ohm's law, the law of heat conduction, the Navier-Stokes equation, or the particle diffusion equation) breaks down and the corresponding transport coefficient becomes irrelevant and meaningless.





Systems: closed and semi-closed

Systems play the same role in statistical mechanics as is played by particles in kinetic theory. A system is any physical entity. (Obviously, this is an exceedingly general concept!) Examples are a galaxy, the Sun, a sapphire crystal, the fundamental mode of vibration of that crystal, an aluminum atom in that crystal, an electron from that aluminum atom, a quantum state in which that electron could reside, . . .

SEMICLOSED SYSTEMS

Statistical mechanics focuses special attention on systems that couple only weakly to the rest of the universe. Stated more precisely, we are interested in systems who relevant internal evolution timescales, $\tau_{\rm int}$ are short compared with the external timescales, $\tau_{\rm ext}$ on which they exchange energy, entropy, particles, and so forth, with their surroundings. Such systems are said to be *semiclosed*, and in the idealized limit where one completely ignores their external interactions, they are said to be closed. The statistical mechanics formalism for dealing with them relies on the assumption $\tau_{int}/\tau_{ext}\ll$ 1; in this sense, it is a variant of a two-lengthscale expansion (Box 3.3).

Some examples will elucidate these concepts. For a galaxy of, say, 10^{11} stars, τ_{int} is the time it takes a star to cross the galaxy, so $\tau_{int} \sim 10^8$ yr. The external timescale is the time since the galaxy's last collison with a neighboring galaxy or the time since it was born by separating from the material that formed neighboring galaxies; both these times are $\tau_{ext}\sim 10^{10}$ yr, so $\tau_{int}/\tau_{ext}\sim 1/100$, and the galaxy is semiclosed. For a small volume of gas inside the Sun (say, 1 m on a side), τ_{int} is the timescale for the constituent electrons, ions, and photons to interact through collisions, $\tau_{int} \lesssim 10^{-10}$ s; this is much smaller than the time for external heat or particles to diffuse from the cube's surface to its center, $\tau_{\rm ext}\gtrsim 10^{-5}\,{\rm s},$ so the cube is semiclosed. An individual atom in a crystal is so strongly coupled to its neighboring atoms by electrostatic forces that $\tau_{int}\sim\tau_{ext}$, which means the atom is not semiclosed. By contrast, for a vibrational mode of the crystal, τ_{int} is the mode's vibration period, and τ_{ext} is the time to exchange energy with other modes and thereby damp the chosen mode's vibrations; quite generally, the damping time is far longer than the period, so the mode is semiclosed. (For a highly polished, cold sapphire crystal weighing several kilograms, τ_{ext} can be ${\sim}10^9\,\tau_{int}.)$ Therefore, it is the crystal's vibrational normal modes and not its atoms that are amenable to the statistical mechanical tools we shall develop.



Ensembles

In kinetic theory, we study statistically a collection of a huge number of particles. Similarly, in statistical mechanics, we study statistically a collection or *ensemble* of a huge number of systems. This ensemble is actually only a conceptual device, a foundation for statistical arguments that take the form of thought experiments. As we shall see, there are many different ways that one can imagine forming an ensemble, and this freedom can be used to solve many different types of problems.

In some applications, we require that all the systems in the ensemble be closed and be identical in the sense that they all have the same number of degrees of freedom, W; are governed by hamiltonians with the same functional forms $H(\mathbf{q}, \mathbf{p})$; and have the same volume V and total internal energy E (or \mathcal{E} , including rest masses). However, the values of the generalized coordinates and momenta at a specific time t, $\{\mathbf{q}(t), \mathbf{p}(t)\}$, need not be the same (i.e., the systems need not be in the same state at time t). If such a conceptual ensemble of identical closed systems (first studied by Boltzmann) evolves until it reaches statistical equilibrium (Sec. 4.5), it then is called *microcanonical*; see Table 4.1.

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	Microcanonical (const. NVE)
TABLE 4.1: Statistical-	equilibrium ensembles used in this chapter
TABLE 4.1: Statistical- Ensemble	equilibrium ensembles used in this chapter Quantities exchanged with surroundings
TABLE 4.1: Statistical- Ensemble Microcanonical	equilibrium ensembles used in this chapter Quantities exchanged with surroundings Nothing
TABLE 4.1: Statistical- Ensemble Microcanonical Canonical	equilibrium ensembles used in this chapter Quantities exchanged with surroundings Nothing Energy <i>E</i>
TABLE 4.1: Statistical- Ensemble Microcanonical Canonical Gibbs	equilibrium ensembles used in this chapter Quantities exchanged with surroundings Nothing Energy E Energy E and volume V

Preliminaries

1. This generalized η is proportional to the number of systems $N_{\rm sys}$ in our ensemble. (If we double $N_{\rm sys}$, then η will double.) Because our ensemble is only a conceptual device, we don't really care how many systems it contains, so we divide η by $N_{\rm sys}$ to get a renormalized, $N_{\rm sys}$ -independent distribution function, $\rho = \eta / N_{\rm sys}$, whose physical interpretation is

 $\rho(t; \mathbf{q}, \mathbf{p}) = \begin{pmatrix} \text{probability that a system, drawn randomly} \\ \text{from our ensemble, will be in a quantum state} \\ \text{at location } (\mathbf{q}, \mathbf{p}) \text{ in phase space at time } t \end{cases}$

(4.4)

2. If the systems of our ensemble can exchange particles with the external universe (as is the case, for example, in the grand canonical ensemble of Table 4.1), then their number of degrees of freedom, *W*, can change, so ρ may depend on *W* as well as on location in the 2*W*-dimensional phase space: $\rho(t; W, \mathbf{q}, \mathbf{p})$.

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Distribution function

In the sector of the system's phase space with W degrees of freedom, denote the number density of quantum states by

$$\mathcal{N}_{\text{states}}(W, \mathbf{q}, \mathbf{p}) = \frac{dN_{\text{states}}}{d^{W}qd^{W}p} \equiv \frac{dN_{\text{states}}}{d\Gamma_{W}}.$$
(4.5)

Here we have used

$$d^{W}q \equiv dq_{1}dq_{2}\cdots dq_{W}, \quad d^{W}p \equiv dp_{1}dp_{2}\cdots dp_{W}, \quad d\Gamma_{W} \equiv d^{W}q \ d^{W}p. \quad (4.6)$$

Then the sum of the occupation probability ρ over all quantum states, which must (by the meaning of probability) be unity, takes the form

$$\sum_{n} \rho_{n} = \sum_{W} \int \rho \mathcal{N}_{\text{states}} d\Gamma_{W} = 1.$$
(4.7)

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GEOMETRICAL VIEWPOINT

Equations (4.4)-(4.7) require some discussion. Just as the events and 4-momenta in relativistic kinetic theory are geometric, frame-independent objects, similarly location in phase space in statistical mechanics is a geometric, coordinate-independent concept (though our notation does not emphasize it). The quantities $\{q, p\} \equiv$ $\{q_1, q_2, \ldots, q_W, p_1, p_2, \ldots, p_W\}$ are the coordinates of that phase-space location. When one makes a canonical transformation from one set of generalized coordinates and momenta to another (Ex. 4.1), the qs and ps change, but the geometric location in phase space does not. Moreover, just as the individual spatial and momentum volumes dV_x and dV_p occupied by a set of relativistic particles in kinetic theory are frame dependent, but their product $dV_x dV_p$ is frame-independent [cf. Eqs. (3.7a)–(3.7c)], so also in statistical mechanics the volumes $d^{W}q$ and $d^{W}p$ occupied by some chosen set of systems are dependent on the choice of canonical coordinates (they change under a canonical transformation), but the product $d^W q d^W p \equiv d\Gamma_W$ (the systems' total volume in phase space) is independent of the choice of canonical coordinates and is unchanged by a canonical transformation. Correspondingly, the number density of states in phase space $N_{\text{states}} = dN_{\text{states}}/d\Gamma_W$ and the statistical mechanical distribution function $\rho(t; W, q, p)$, like their kinetic-theory counterparts, are geometric, coordinateindependent quantities: they are unchanged by a canonical transformation. See Ex. 4.1 and references cited there.

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DENSITY OF STATES

Classical thermodynamics was one of the crowning achievements of nineteenthcentury science. However, thermodynamics was inevitably incomplete and had to remain so until the development of quantum theory. A major difficulty, one that we have already confronted in Chap. 3, was how to count the number of states available to a system. As we saw in Chap. 3, the number density of quantum mechanical states in the 6-dimensional, single-particle phase space of kinetic theory is (ignoring particle spin) $\mathcal{N}_{\text{states}} = 1/h^3$, where *h* is Planck's constant. Generalizing to the 2*W*-dimensional phase space of statistical mechanics, the number density of states turns out to be $1/h^W$ [one factor of 1/h for each of the canonical pairs $(q_1, p_1), (q_2, p_2), \cdots, (q_W, p_W)$]. Formally, this follows from the canonical quantization procedure of elementary quantum mechanics.

When the laws of

quantum mechanics were developed, it became clear that all identical particles are indistinguishable, so having particle 1 at location A in phase space and an identical particle 2 at location B must be counted as the same state as particle 1 at B and particle 2 at A. Correspondingly, if we attribute half the quantum state to the classical phase-space location {1 at A, 2 at B} and the other half to {1 at B, 2 at A}, then the classical number density of states per unit volume of phase space must be reduced by a factor of 2—and more generally by some *multiplicity factor* M. In general, therefore, we can write the actual number density of states in phase space as

$$\mathcal{N}_{\text{states}} = \frac{dN_{\text{states}}}{d\Gamma_W} = \frac{1}{\mathcal{M}h^W},$$
(4.8a)

and correspondingly, we can rewrite the normalization condition (4.7) for our probabilistic distribution function as

$$\boxed{\sum_{n} \rho_{n} \equiv \sum_{W} \int \rho \mathcal{N}_{\text{states}} d\Gamma_{W} = \sum_{W} \int \rho \frac{d\Gamma_{W}}{\mathcal{M}h^{W}} = 1.}$$
(4.8b)

This equation can be regarded, in the classical domain, as defining the meaning of the sum over states n. We shall make extensive use of such sums over states.

For N i that $\mathcal{M} = i$ can be rega the phase s \mathcal{M} (the nu	dentical and V!. If we inclu arded as dege space of each imber of diff	indistinguishable particles with zero spin, it is not de the effects of quantum mechanical spin (and the nerate), then there are g_1 [Eq. (3.16)] more states particle than we thought, so an individual state's ferent phase-space locations to be attributed to the	hard to see spin states present in nultiplicity ne state) is
reduced to			
	$\mathcal{M} = \frac{N!}{g_s^N}$	for a system of N identical particles with spin s.	(4.8c)

This is the quantity that appears in the denominator of the sum over states [Eq. (4.8b)].

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ENSEMBLE AVERAGE

Each system in an ensemble is endowed with a total energy that is equal to its hamiltonian, $E = H(\mathbf{q}, \mathbf{p})$ [or relativistically, $\mathcal{E} = H(\mathbf{q}, \mathbf{p})$]. Because different systems reside at different locations (\mathbf{q}, \mathbf{p}) in phase space, they typically will have different energies. A quantity of much interest is the *ensemble-averaged energy*, which is the average value of *E* over all systems in the ensemble:

$$\langle E \rangle = \sum_{n} \rho_{n} E_{n} = \sum_{W} \int \rho E \mathcal{N}_{states} d\Gamma_{W} = \sum_{W} \int \rho E \frac{d\Gamma_{W}}{\mathcal{M}h^{W}}.$$
 (4.10a)

For any other function $A(\mathbf{q}, \mathbf{p})$ defined on the phase space of a system (e.g., the linear momentum or the angular momentum), one can compute an ensemble average by the obvious analog of Eq. (4.10a):

$$\langle A \rangle = \sum_{n} \rho_n A_n. \tag{4.10b}$$

Our probabilistic distribution function $\rho_n = \rho(t; \mathbf{W}, \mathbf{q}, \mathbf{p})$ has deeper connections to quantum theory than the above discussion reveals. In the quantum domain, even if we start with a system whose wave function ψ is in a *pure* state (ordinary, everyday type of quantum state), the system may evolve into a *mixed state* as a result of (i) interaction with the rest of the universe and (ii) our choice not to keep track of correlations between the universe and the system (Box 4.2 and Sec. 4.7.2). The system's initial, pure state can be described in geometric, basis-independent quantum language by a state vector ("ket") $|\psi\rangle$; but its final, mixed state requires a different kind of quantum description: a *density operator* $\hat{\rho}$ becomes our classical probabilistic distribution function $\rho(t, W, \mathbf{q}, \mathbf{p})$; see Box 4.2 for some details.

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The time derivative on the left is now taken moving through phase space with a fiducial system that does not interact with the external universe.

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STATISTICAL EQUILIBRIUM AND JEANS' THEOREM

Consider an ensemble of identical systems, all of which have the same huge number of degrees of freedom (dimensionality $W \gg 1$). Put all the systems initially in the same state, and then let them exchange heat (but not particles, volume, or anything else) with an external thermal bath that has a huge heat capacity and is in thermodynamic equilibrium at some temperature T. (For example, the systems might be impermeable cubes of gas 1 km on a side near the center of the Sun, and the thermal bath might be all the surrounding gas near the Sun's center; or the systems might be identical sapphire crystals inside a huge cryostat, and the thermal bath might be the cryostat's huge store of liquid helium.) After a sufficiently long time, $t \gg \tau_{ext}$, the ensemble will settle down into equilibrium with the bath (i.e., it will become the canonical ensemble mentioned in Table 4.1 above). In this final, canonical equilibrium state, the probability $\rho(t, \mathbf{q}, \mathbf{p})$ is independent of time t, and it no longer is affected by interactions with the external environment. In other words, the interaction terms in the evolution equation (4.16) have ceased to have any net effect: on average, for each interaction event that feeds energy into a system, there is an interaction event that takes away an equal amount of energy. The distribution function, therefore, satisfies the interaction-free, collisionless Boltzmann equation (4.15) with the time derivative $\partial \rho / \partial t$ removed:

$$[\rho, H]_{\mathbf{q}, \mathbf{p}} \equiv \frac{\partial \rho}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial \rho}{\partial p_j} \frac{\partial H}{\partial q_j} = \mathbf{0}. \tag{4.17}$$

We use the phrase *statistical equilibrium* to refer to any ensemble whose distribution function has attained such a state and thus satisfies Eq. (4.17).

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To summarize, an ensemble of identical systems with many degrees of freedom $W\gg$ 1, which have reached statistical equilibrium by exchanging energy but nothing else with a huge thermal bath, has the following canonical distribution function:

 $\rho_{\text{canonical}} = C \exp(-\mathcal{E}/k_B T), \quad \rho_{\text{canonical}} = C' \exp(-E/k_B T) \text{ nonrelativistically.}$

Here $\mathcal{E}(\mathbf{q},\,\mathbf{p})$ is the energy of a system at location $\{\mathbf{q},\,\mathbf{p}\}$ in phase space, k_B is Boltzmann's constant, T is the temperature of the heat bath, and C is whatever normalizamany constants r is the temperature of the har bar, and c is which for many static formation is required to guarantee that $\sum_n \rho_n = 1$. The normalityistic expression is obtained by removing all the particle rest masses from the total energy \mathcal{E} and then taking the low-temperature, low-thermal-velocities limit.

(4.20)

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GENERAL EQUILIBRIUM ENSEMBLE

We can easily generalize the canonical distribution to an ensemble of systems that exchange other additive conserved quantities (extensive variables) K_1, K_2, \ldots , in addition to energy \mathcal{E} , with a huge, thermalized bath. By an obvious generalization of the argument in Sec. 4.4.1, the resulting statistical equilibrium distribution function must have the form

$$\rho = C \exp\left(-\beta \mathcal{E} - \sum_{A} \beta_{A} K_{A}\right). \tag{4.21}$$

When the extensive variables K_A that are exchanged with the bath (and thus appear explicitly in the distribution function ρ) are energy \mathcal{E} , momentum P, angular momentum J, the number N_I of the species I of conserved particles, volume V, or any combination of these quantities, it is conventional to rename the multiplicative factors β and β_A so that ρ takes on the form

$$\rho = C \exp\left[\frac{-\mathcal{E} + \mathbf{U} \cdot \mathbf{P} + \mathbf{\Omega} \cdot \mathbf{J} + \sum_{I} \tilde{\mu}_{I} N_{I} - PV}{k_{B}T}\right].$$
(4.22)

Here T, U, Ω , $\tilde{\mu}_I$, and P are constants (called *intensive* variables) that are the same for all systems and subsystems (i.e., that characterize the full ensemble and all its subensembles and therefore must have been acquired from the bath); any extensive variable that is not exchanged with the bath must be omitted from the exponential and be replaced by an implicit delta function.

SPECIAL EQUILIBRIUM ENSEMBLES

Henceforth (except in Sec. 4.10.2, when discussing black-hole atmospheres), we restrict our baths always to be at rest in our chosen reference frame and to be nonrotating with respect to inertial frames, so that $\mathbf{U} = \mathbf{\Omega} = 0$. The distribution function ρ can then either be a delta function in the system momentum **P** and angular momentum **J** (if momentum and angular momentum are not exchanged with the bath), or it can involve no explicit dependence on **P** and **J** (if momentum and angular momentum are exchanged with the bath; cf. Eq. (4.22) with $\mathbf{U} = \mathbf{\Omega} = 0$). In either case, if energy is the only other quantity exchanged with the bath, then the distribution function is the canonical one [Eq. (4.20)]:

$$\rho_{\text{canonical}} = C \exp\left[\frac{-\mathcal{E}}{k_B T}\right] = C' \exp\left[\frac{-E}{k_B T}\right],$$
(4.25a)

where (obviously) the constants C and C' are related by

$$C' = C \exp\left[-\sum_{I} N_{I} m_{I} / k_{B} T\right].$$

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$$\rho_{\text{Gibbs}} = C \exp\left[\frac{-(\mathcal{E} + PV)}{k_B T}\right] = C' \exp\left[\frac{-(E + PV)}{k_B T}\right]$$
(4.25b)

(with an implicit delta function in N_I and possibly in J and P). The combination $\mathcal{E} + PV$ is known as the *enthalpy* H. If the exchanged quantities are energy and particles but not volume (e.g., if the systems are 1-m cubes inside the Sun with totally imaginary walls through which particles and heat can flow), then the equilibrium is the *grand canonical ensemble*, with

$$\rho_{\text{grand canonical}} = C \exp\left[\frac{-\mathcal{E} + \sum_{I} \tilde{\mu}_{I} N_{I}}{k_{B}T}\right] = C \exp\left[\frac{-E + \sum_{I} \mu_{I} N_{I}}{k_{B}T}\right]$$
(4.25c)

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SINGLE-PARTICLE QUANTUM STATES (MODES)

As an important example, let each system be a single-particle quantum state of some field. These quantum states can exchange particles (quanta) with one another. As we shall see, in this case the above considerations imply that, in sta-Using the set of the ter [Eqs. (3.22a), (3.22b)]. Our derivation of these mean occupation numbers will

Choose one specific mode ${\mathcal S}$ [e.g., a nonrelativistic electron plane-wave mode in a box of side L with spin up and momentum $\mathbf{p} = (5, 3, 17)h/L$]. There is one such mode ${\mathcal S}$ in each of the systems in our ensemble, and these modes (all identical in their properties) form a subensemble of our original ensemble. Our derivation focuses on this subensemble of identical modes ${\cal S}.$ Because each of these modes can exchange energy and particles with all the other modes in its system, the subensemble is grand canonically distributed.

The (many-particle) quantum states allowed for mode S are states in which Scontains a finite number *n* of particles (quanta). Denote by $\mathcal{E}_{\mathcal{S}}$ the energy of one particle residing in mode \mathcal{S} . Then the mode's total energy when it is in the state $|n\rangle$ (when it contains *n* quanta) is $\mathcal{E}_n = n\mathcal{E}_S$. [For a freely traveling, relativistic electron (index $\xi_{S} = \sqrt{m^2 + p^2}$, Eq. (1.40), where p is the mode's momentum, $p_z = jh/lar$ for some integer j and similarly for p_y and p_{zi} for a phonon mode with angular eigenfrequency of vibration ω , $\mathcal{E}_{S} = \hbar\omega$.] Since the distribution of the ensemble's modes among the allowed quantum states is grand canonical, the probability ρ_n of being in state $|n\rangle$ is [Eq. (4.25c)]

$$\rho_n = C \exp\left(\frac{-\mathcal{E}_n + \tilde{\mu}n}{k_B T}\right) = C \exp\left(\frac{n(\tilde{\mu} - \mathcal{E}_S)}{k_B T}\right), \quad (4.26)$$

where $\tilde{\mu}$ and T are the chemical potential and temperature of the bath of other modes, with which the mode S interacts.⁸



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 $k_{\rm B}T$ 0.5 106

. (4.27a)

(4.27b)



BOSON MODES: BOSE-EINSTEIN DISTRIBUTION

Suppose that S is a boson mode (i.e., its particles have integral spin), so it can contain any nonnegative number of quanta; that is, n can assume the values 0, 1, 2, 3, Then the normalization condition $\sum_{n=0}^{\infty} \rho_n = 1$ fixes the constant in the grand canonical distribution (4.26), resulting in

$$\rho_n = \left[1 - \exp\left(\frac{\tilde{\mu} - \mathcal{E}_S}{k_B T}\right)\right] \exp\left(\frac{n(\tilde{\mu} - \mathcal{E}_S)}{k_B T}\right).$$

From this grand canonical distribution we can deduce the mean number of bosons in mode S:

$$\eta_{\mathcal{S}} \equiv \langle n \rangle = \sum_{n=1}^{\infty} n\rho_n = \frac{1}{\exp[(\mathcal{E}_{\mathcal{S}} - \tilde{\mu})/(k_B T)] - 1} = \frac{1}{\exp[(E_{\mathcal{S}} - \mu)/(k_B T)] - 1},$$
(4.28b)

in accord with Eq. (3.22b). As for fermions, this Bose-Einstein mean occupation number and underlying grand canonical distribution (4.28a) are valid generally, and not solely for the freely moving bosons of Chap. 3.

When the mean occupation number is small, $\eta_S \ll 1$, both the bosonic and the fermionic distribution functions are well approximated by the classical Boltzmann mean occupation number

$$\eta_{\rm S} = \exp[-(\mathcal{E}_{\mathcal{S}} - \tilde{\mu})/(k_B T)].$$

In Sec. 4.9 we explore an important modern application of the Bose-Einstein mean occupation number (4.28b): Bose-Einstein condensation of bosonic atoms in a magnetic trap.



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4.4.4 Equipartition Theorem for Quadratic, Classical Degrees of Freedom

As a second example of statistical equilibrium distribution functions, we derive the

classical equipartition theorem using statistical methods. To motivate this theorem, consider a diatomic molecule of nitrogen, N_2 . To a good approximation, its energy (its hamiltonian) can be written as

$$E = \frac{p_x^2}{2M} + \frac{p_y^2}{2M} + \frac{p_z^2}{2M} + \frac{P_\ell^2}{2M_\ell} + \frac{1}{2}M_\ell\,\omega_v^2\,\ell^2 + \frac{J_x^2}{2I} + \frac{J_y^2}{2I}.$$
 (4.3)

Here M is the molecule's mass; p_x , p_y , and p_z are the components of its translational momentum; and the first three terms are the molecule's kinetic energy of translation. The next two terms are the molecule's longitudinal vibration energy, with ℓ the change of the molecule's length (change of the separation of its two nuclei) from equilibrium, P_ℓ the generalized momentum conjugate to that length change, ω_v the vibration frequency, and M_{ℓ} the generalized mass associated with that vibration. The last two terms are the molecule's energy of end-over-end rotation, with J_x and J_y the components of angular momentum associated with this two-dimensional rotator and I its moment of inertia

Notice that every term in this hamiltonian is quadratic in a generalized coordinate or generalized momentum! Moreover, each of these coordinates and momenta appears only in its single quadratic term and nowhere else, and the density of states is independent of the value of that coordinate or momentum. We refer to such a coordinate or momentum as a *quadratic degree of freedom*. In some cases (e.g., the vibrations and rotations but not the translations), the en-

ergy $E_\xi=\alpha\xi^2$ of a quadratic degree of freedom ξ is quantized, with some energy separation ε_0 between the ground state and first excited state (and with energy separations to higher states that are $\leq \varepsilon_0$). If (and only if) the thermal energy $k_B T$ is significantly larger than ε_0 , then the quadratic degree of freedom ζ will be excited far above its ground state and will behave classically. The equipartition theorem applies only at these high temperatures. For diatomic nitrogen, the rotational degrees of freedom J_x and J_y have $\varepsilon_0 \sim 10^{-4}$ eV and $\varepsilon_0/k_B \sim 1$ K, so temperatures big compared to 1 K are required for J_x and J_y to behave classically. By contrast, the vibrational degrees of freedom ℓ and P_{ℓ} have $\varepsilon_0 \sim 0.1$ eV and $\varepsilon_0/k_B \sim 1,000$ K, so temperatures of a few thousand Kelvins are required for them to behave classically. Above ${\sim}10^4$ K, the hamiltonian (4.30) fails: electrons around the nuclei are driven into excited states. and the molecule breaks apart (dissociates into two free atoms of nitrogen).

(4.29)

The equipartition theorem holds for any classical, quadratic degree of freedom [i.e., at temperatures somewhat higher than $T_o = \varepsilon_o/(k_B T)$]. We derive this theorem using the canonical distribution (4.25a). We write the molecule's total energy as $E = \alpha \xi^2 + E'$, where E' does not involve ξ . Then the mean energy associated with ξ is

$$\langle E_{\xi} \rangle = \frac{\int \alpha \xi^2 \ e^{-\beta(\alpha \xi^2 + E')} d\xi \ d(\text{other degrees of freedom})}{\int \ e^{-\beta(\alpha \xi^2 + E')} d\xi \ d(\text{other degrees of freedom})}. \tag{4.31}$$

Here the exponential is that of the canonical distribution function (4.25a), the denominator is the normalizing factor, and we have set $\beta \equiv 1/(k_BT)$. Because ξ does not appear in the portion $E^{'}$ of the energy, its integral separates out from the others in both numerator and denominator, and the integrals over E^{\prime} in numerator and denominator cancel. Rewriting $\int \alpha \xi^2 \exp(-\beta \alpha \xi^2) d\xi$ as $-d/d\beta [\int \exp(-\beta \alpha \xi^2) d\xi]$, Eq. (4.31) becomes

$$\langle E_{\xi} \rangle = -\frac{d}{d\beta} \ln \left[\int \exp(-\beta \alpha \xi^2) d\xi \right]$$

= $-\frac{d}{d\beta} \ln \left[\frac{1}{\sqrt{\beta \alpha}} \int du e^{-u^2} du \right] = \frac{1}{2\beta} = \frac{1}{2} k_B T.$ (4.32)

Therefore, in statistical equilibrium, the mean energy associated with any classical, quadratic degree of freedom is $\frac{1}{2}k_BT$. This is the equipartition theorem. Note that the factor $\frac{1}{2}$ follows from the quadratic nature of the degrees of freedom.

For our diatomic molecule, at room temperature there are three translational and two rotational classical, quadratic degrees of freedom $(p_x, p_y, p_z, J_x, J_y)$, so the mean total energy of the molecule is $\frac{5}{2}k_BT$. At a temperature of several thousand Kelvins, the two vibrational degrees of freedom, ℓ and P_{ℓ} , become classical and the molecule's mean total energy is $\frac{7}{2}k_BT$. Above ~10⁴ K the molecule dissociates, and its two parts (the two nitrogen atoms) have only translational quadratic degrees of freedom, so the mean energy per atom is $\frac{3}{3}k_BT$.

Translational, rotational and vibrational degrees of freedom

Motion	Structure	Degrees of freedom	Average energy
Translation	All	3	$\frac{3}{2}kT$
	Linear	2	kT
Rotation	Non-linear	3	$\frac{3}{2}kT$
Vibration	Linear	3N - (3 + 2) = 3N - 5	$2(3N-5)\frac{1}{2}kT$
	Non-linear	3N - (3 + 3) = 3N - 6	$2(3N-6)\frac{1}{2}kT$
Total	Linear	3 <i>N</i>	$\left(3N-\frac{5}{2}\right)kT$
	Non-linear	3N	3(N-1)kT



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4.6 The Ergodic Hypothesis

The ensembles we have been studying are almost always just conceptual ones that do not exist in the real universe. We have introduced them and paid so much attention to them not for their own sakes, but because, in the case of statistical-equilibrium ensembles, they can be powerful tools for studying the properties of a single, individual system that really does exist in the universe or in our laboratory.

This power comes about because a sequence of snapshots of the single system, taken at times separated by sufficiently large intervals Δt , has a probability distribution ρ (for the snapshots' instantaneous locations $\{q, p\}$ in phase space) that is the same as the distribution function ρ of some conceptual, statistical-equilibrium ensemble. If the single system is closed, so its evolution is driven solely by its own hamiltonian, then the time between snapshots should be $\Delta t \gg \tau_{\rm intr}$, and its snapshots will be (very nearly) microcanonically distributed. If the single system exchanges energy, and only energy, with a thermal bath on a timescale $\tau_{\rm ext}$, then the time between snapshots should be $\Delta t \gg \tau_{\rm ext}$, and its snapshots will be canonically distributed; similarly for the other types of bath interactions. This property of snapshots is equivalent to the statement that for the individual system, the long-term time average¹⁰ of any function of the system's location in phase space is equal to the statistical-equilibrium ensemble average:

$$\bar{A} \equiv \lim_{T \to \infty} \frac{1}{T} \int_{-T/2}^{+T/2} A(\mathbf{q}(t), \mathbf{p}(t)) = \langle A \rangle \equiv \sum_{n} A_{n} \rho_{n}.$$

(4.33)

This property comes about because of *ergodicity*: the individual system, as it evolves, visits each accessible quantum state n for a fraction of the time that is equal to the equilibrium ensemble's probability ρ_n .









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<text><text><text><text><text><text>



As time passes each system evolves under the action of the systems' common hamiltonian. As depicted in Fig. 4.2b, this evolution distorts the occupied region of phase space; but Liouville's theorem dictates that the occupied region's volume remain unchanged and, correspondingly, that the ensemble's entropy remains unchanged.

$$S = -k_B \int (\rho \ln \rho) \mathcal{N}_{\text{states}} d\Gamma = k_B \ln(\mathcal{N}_{\text{states}} \Delta \Gamma)$$

How can this be so? The ensemble is supposed to evolve into statistical equilibrium, with its distribution function uniformly spread out over that entire portion of phase space allowed by the hamiltonian's constants of motion—a portion of phase space far, far larger —and in the process the entropy is supposed to increase.

Coarsening

Figure 4.2b,c resolves the paradox. As time passes, the occupied region becomes more and more distorted. It retains its phase-space volume, but gets strung out into a winding, contorted surface (Fig. 4.2b), which (by virtue of the ergodic hypothesis) ultimately passes arbitrarily close to any given point in the region allowed by the constants of motion. This ergodic wandering is called phase mixing. Ultimately, the physicist gets tired of keeping track (or ceases to be able to keep track) of all these contortions of the occupied region and chooses instead to take a coarse-grained viewpoint that averages over scales larger than the distance between adjacent portions of the occupied surface, and thereby regards the ensemble as having become spread over the entire allowed region (Fig. 4.2c). More typically, the physicist will perform a coarsegrained smearing out on some given, constant scale at all times. Once the transverse scale of the ensemble's lengthening and narrowing phase-space region drops below the smearing scale, its smeared volume and its entropy start to increase. Thus, for an ensemble of closed systems it is the physicist's choice (though often a practical necessity) to perform coarse-grain averaging that causes entropy to increase and causes the ensemble to evolve into statistical equilibrium.

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Discarding correlations

When one reexamines these issues in quantum mechanical language, one discovers that the entropy increase is caused by the physicist's discarding the quantum mechanical correlations (the off-diagonal terms in the density matrix of Box 4.2) that get built up through the systems' interaction with the rest of the universe. This discarding of correlations is accomplished through a trace over the external universe's basis states (Box 4.2), and if the state of system plus universe was originally pure, this tracing (discarding of correlations) makes it mixed. From this viewpoint, then, *it is the physicist's choice to discard correlations with the external universe that causes the entropy increase and the evolution toward statistical equilibrium*. Heuristically, we can say that the entropy does not increase until the physicist actually (or figuratively) chooses to let it increase by ignoring the rest of the universe. For a simple example, see Box 4.3 and Ex. 4.9.



4.10 Statistical Mechanics in the Presence of Gravity 12

Systems with significant gravity behave quite differently in terms of their statistical mechanics than do systems without gravity. This has led to much controversy as to whether statistical mechanics can really be applied to gravitating systems. Despite that controversy, statistical mechanics has been applied in the presence of gravity in a variety of ways, with great success, resulting in important, fundamental conclusions. In this section, we sketch some of those applications: to galaxies, black holes, the universe as a whole, and the formation of structure in the universe. Our discussion is intended to give just the flavor of these subjects and not full details, so we state some things without derivation. This is necessary in part because many of the phenomena we describe rely for their justification on general relativity (Part VII) and/or quantum field theory in curved spacetime (see, e.g., Parker and Toms, 2009).

Galaxies as closed systems of non-interacting stars



 $\tau_{\rm int} \sim 2R/v \sim 10^8$ yr.

4.10.1 Galaxies 12

A galaxy is dominated by a roughly spherical distribution of dark matter (believed to comprise elementary particles with negligible collision cross section) with radius $R_D \sim 3 \times 10^{21}$ m and mass $M_D \sim 10^{12}$ kg. The dark matter and roughly $N \sim 10^{11}$ stars, each with fiducial mass $m \sim 10^{30}$ kg, move in a common gravitational potential well. (As we discuss in Chap. 28, the ratio of regular, or baryonic, matter to dark matter is roughly 1:5 by mass.) The baryons (stars plus gas) are mostly contained within a radius $R \sim 3 \times 10^{30}$ m. The characteristic speed of the dark matter and the stars and gas is $v \sim (GM_D/R_D)^{1/2} \sim (GNm/R_D)^{1/2} \sim 200 \, {\rm km} \, {\rm s}^{-1}$. For the moment, focus on the stars, with total mass M = Nm, ignoring the dark matter and gas, whose presence does not change our conclusions.

Age of galaxy 0^{10} yr. Galaxies have distant encounters with their neighbors on timescales that can be smaller than their ages but still much longer than τ_{ini} ; in this sense, they can be thought of as semiclosed systems weakly coupled to their environments. In this subsection, we idealize our chosen galaxy as fully closed (no interaction with its environment). Direct collisions between stars are exceedingly rare, and strong two-star gravitational encounters, which happen when the impact parameter¹⁵ is smaller than $\sim Gm/v^2 \sim R/N$, are also negligibly rare except, sometimes, near the center of a galaxy (which we ignore until the last paragraph of this subsection). We can therefore regard each of the galaxy's stars as moving in a gravitational potential determined by the smoothed-out mass of the dark matter and all the other stars, and can use Hamiltonian dynamics to describe their motions.

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Entropy of a galaxy	
Probability density of N stars	Are galaxies at equilibrium ?
Imagine that we have an ensemble of such galaxies, all with the same number of stars <i>N</i> , the same mass <i>M</i> , and the same energy <i>E</i> (in a tiny range δE). We begin our study of that ensemble by making an order-of-magnitude estimate of the probability ρ of finding a chosen galaxy from the ensemble in some chosen quantum state. We compute that probability from the corresponding probabilities for its subsystems, individual stars. The phase-space volume available to each star in the galaxy is $\sim R^3(mv)^3$, the density of single-particle quantum states (modes) in each star's phase space is $1/h^3$, the number of available modes is the product of these, $\sim (Rmv/h)^3$, and the probability of the star occupying the chosen mode, or any other mode, is the reciprocal of this product, $\sim /h/(Rmv)^3$. The probability for mean stars (modes) in each stars phase space is the probability of the star occupying the chosen mode, or any other mode, is the reciprocal of this product, $\sim /h/(Rmv)^3$. The probability of the galaxy occupying a state in its phase space is the product of the probability of the stars (modes) is the galaxy occupying a state in its phase space is the product of the probability of the galaxy occupying the chosen mode, or any other mode, is [Eq. (4.18c)]:	Are real galaxies in statistical equilibrium? To gain insight into this question, we estimate the entropy of a galaxy in our ensemble and then ask whether that entropy has any chance of being the maximum value allowed to the galaxy's stars (as it must be if the galaxy is in statistical equilibrium). To briously, the stars (by contrast with electrons) are distinguishable, so we can assume multiplicity $\mathcal{M} = 1$ when estimating the galaxy's entropy. Ignoring the (negligible) correlations among stars, the entropy computed by integating ρ in ρ over the galaxy's full $6N$ -dimensional phase space to your control of the star statistical equilibrium, where $\Delta\Gamma$ is the phase-space volume over which the star wanders in its ergodic, hamiltonian-induced motion (i.e., the phase space volume available to the star). We express this entropy in terms of the galaxy's total mass M and its total nonrel-ativistic energy $E \sim -GM^2/(2E)$ as follows. Since the characteristic stellar speed is $\nu \sim (GM/R)^{1/2}$, the volume of phase space over which the star wanders is $\Delta\Gamma \sim (mv)^3 R^3 \sim (GMm^2R)^{3/2} \sim (-G^2M^3m^2/(2E))^{3/2}$, and the entropy is therefore $S_{\text{Calaxy}} \sim (M/m)k_B \ln(\Delta\Gamma/h^3) \sim (3M/(2m))k_B \ln(-G^2M^3m^2/(2Eh^2))$. (4.58)
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The galaxy entropy increases

Is this the maximum possible entropy available to the galaxy, given the constraints that its mass be M and its nonrelativistic energy be E? No. Its entropy can be made larger by removing a single star from the galaxy to radius $r \gg R$, where the star's energy is negligible. The entropy of the remaining stars will decrease slightly, since the mass M diminishes by m at constant E. However, the entropy associated with the removed star, $\sim(3/2) \ln(GMm^2r/h^2)$, can be made arbitrarily large by making its orbital radius r arbitrarily large. By this thought experiment, we discover that galaxies cannot be in a state of maximum entropy at fixed E and M; they therefore cannot be in a true state of statistical equilibrium.¹⁶ (One might wonder whether there is entropy associated with the galaxy's gravitational field, some of which is due to the stars, and whether that entropy invalidates our analysis. The answer is no. The gravitational field has no randomness, beyond that of the stars themselves, and thus no entropy; its structure is uniquely determined, via Newton's gravitational field equation, by the stars' spatial distribution.)



4.10.2 Black Holes 12

Quantum field theory predicts that, near the horizon of a black hole, the vacuum fluctuations of quantized fields behave thermally, as seen by stationary (non-infalling) observers. More specifically, such observers see the horizon surrounded by an atmosphere that is in statistical equilibrium (a thermalized atmosphere) and that rotates with the same angular velocity Ω_H as the hole's horizon. This remarkable conclusion, due to Stephen Hawking (1976), William Unruh (1976), and Paul Davies (1977), is discussed pedagogically in books by Thorne, Price, and MacDonald (1986) and Frolov and Zelnikov (2011), and more rigorously in a book by Wald (1994). The atmosphere contains all types of particles that can exist in Nature. Very few of the particles manage to escape from the hole's gravitational pull; most emerge from the horizon, fly up to some maximum height, then fall back down to the horizon. Only if they start out moving almost vertically upward (i.e., with nearly zero angular momentum) do they have any hope of escaping. The few that do escape make up a tiny trickle of Hawking radiation (Hawking, 1975) that will ultimately cause the black hole to evaporate, unless it grows more rapidly due to infall of material from the external universe (which it will unless the black hole is far less massive than the Sun).

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In discussing the distribution function for the hole's thermalized, rotating atmosphere, one must take account of the fact that the locally measured energy of a particle decreases as it climbs out of the hole's gravitational field (Ex. 26.4). One does so by attributing to the particle the energy that it would ultimately have if it were to escape from the hole's gravitational grip. This is called the particle's "redshifted energy" and is denoted by \mathcal{E}_{∞} . This \mathcal{E}_{∞} is conserved along the particle's world line, as is the projection $\mathbf{j} \cdot \hat{\mathbf{\Omega}}_H$ of the particle's orbital angular momentum \mathbf{j} along the hole's spin axis (unit direction $\hat{\mathbf{\Omega}}_H$).

The hole's horizon behaves like the wall of a blackbody cavity. Into each upgoing mode (single-particle quantum state) *a* of any and every quantum field that can exist in Nature, it deposits particles that are thermalized with (redshifted) temperature T_H , vanishing chemical potential, and angular velocity Ω_H . As a result, the mode's distribution function—which is the probability of finding N_a particles in it with net redshifted energy $\mathcal{E}_{a\,\infty} = N_a \times$ (redshifted energy of one quantum in the mode) and with net axial component of angular momentum $\mathbf{j}_a \cdot \hat{\mathbf{\Omega}}_H = N_a \times$ (angular momentum of one quantum in the mode)—is

$$\rho_a = C \, \exp\left[\frac{-\mathcal{E}_{a\,\infty} + \mathbf{\Omega}_H \cdot \mathbf{j}_a}{k_B T_H}\right] \tag{4.59}$$

The temperature T_H and angular velocity Ω_H , like all properties of a black hole, are determined completely by the hole's spin angular momentum J_H and its mass M_H . To within factors of order unity, they have magnitudes [Ex. 26.16 and Eq. (26.77)]

$$T_{H} \sim \frac{\hbar}{8\pi k_{B} G M_{H}/c^{3}} \sim \frac{6 \times 10^{-8} \,\mathrm{K}}{M_{H}/M_{\odot}}, \quad \Omega_{H} \sim \frac{J_{H}}{M_{H} (2 G M_{H}/c^{2})^{2}}. \tag{4.60}$$

For a very slowly rotating hole the "~" becomes an "=" in both equations. Notice how small the hole's temperature is, if its mass is greater than or of order M_{\odot} . For such holes the thermal atmosphere is of no practical interest, though it has deep implications for fundamental physics. Only for tiny black holes (that might conceivably have been formed in the big bang) is T_H high enough to be physically interesting.

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First law of thermodynamics & BH Entropy

Suppose that the black hole evolves much more rapidly by accreting matter than by emitting Hawking radiation. Then the evolution of its entropy can be deduced from the first law of thermodynamics for its atmosphere. By techniques analogous to some developed in the next chapter, one can argue that the atmosphere's equilibrium distribution (4.59) implies the following form for the first law (where we set c = 1):

 $dM_{H} = T_{H}dS_{H} + \Omega_{H} \cdot d\mathbf{J}_{H}$ (4.61)

[cf. Eq. (26.92)]. Here dM_H is the change of the hole's mass due to the accretion (with each infalling particle contributing its \mathcal{E}_{∞} to dM_H), dJ_H is the change of the hole's spin angular momentum due to the accretion (with each infalling particle contributing its j), and dS_H is the increase of the black hole's entropy. Because this first law can be deduced using the techniques of statistical mechanics

Because this first and call be deduced using the testingues of statistical interlaints: (Chap. 5), it can be argued (e.g., Zurek and Thorne, 1985) that the hole's entropy increase has the standard statistical mechanical origin and interpretation: if N_{states} is the total number of quantum states that the infalling material could have been in (subject only to the requirement that the total infalling mass-energy be dM_H and total infalling angular momentum be dJ_H), then $dS_H = k_B \log N_{states}$ (cf. Eq. (4.35)]. In other words, the hole's entropy increases by k_B times the logarithm of the number of quantum mechanically different ways that we could have produced its changes of mass and angular momentum, dM_H and dJ_H . Correspondingly, we can regard the hole's total entropy as k_B times the logarithm of the number of ways in which it could have been made. That number of ways is enormous, and correspondingly, the hole's entropy is enormous. This analysis, when carried out in full detail (Zurek and Thorne, 1985), reveals that the entropy is [Eq. (26.93)]

$$S_H = k_B \frac{A_H}{4L_P^2} \sim 1 \times 10^{77} k_B \left(\frac{M_H}{M_\odot}\right)^2,$$
 (4.62)

where $A_H\sim 4\pi (2GM_H/c^2)$ is the surface area of the hole's horizon, and $L_P=\sqrt{G\hbar/c^3}=1.616\times 10^{-33}\,{\rm cm}$ is the Planck length—a result first proposed by Bekenstein (1972) and first proved by Hawking (1975).

What is it about a black hole that leads to this peculiar thermal behavior and enormous entropy? Why is a hole so different from a star or galaxy? The answer lies in the black-hole horizon and the fact that things that fall inward through the horizon cannot get back out. From the perspective of quantum field theory, the horizon produces the thermal behavior. From that of statistical mechanics, the horizon produces the loss of information about how the black hole was made and the corresponding entropy increase. In this sense, the horizon for a black hole plays a role analogous to coarse-graining in conventional classical statistical mechanics.¹⁷









More on Black Hole Thermodynamics & SM (D. Wallace)

In this article, and its sequel, I want to lay out as carefully and thoroughly as I can the theoretical evidence for BHT. It is written with the zeal of the convert: I began this project sharing at least some of the outsiders' scepticism, and became persuaded that the evidence is enormously strong both that black holes are thermodynamical systems in the fullest sense of the word, and that their thermodynamic behaviour has a statistical-mechanical underpinning in quantum gravity (and, as a consequence, that black hole evaporation is a unitary process not different in kind from the cooling of other hot systems, and that it involves no fundamental loss of information).

Black hole thermodynamics (BHT) is perhaps the most striking and unexpected development in the theoretical physics of the last forty years. It combines the three main areas of 'fundamental' theoretical physics — quantum theory, general relativity, and thermal physics — and it offers a conceptual testing ground for quantum gravity that might be the nearest that field has to experimental evidence. Yet BHT itself relies almost entirely on theoretical arguments, and its most celebrated result — Hawking's argument that black holes emit radiation — has no direct empirical support and little prospect of getting any. So to outsiders — to physicists in other disciplines, or to philosophers of science — the community's confidence in BHT can seem surprising, or even suspicious. Can

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4.10.3 The Universe 12

Observations and theory agree that the universe, when far younger than 1 s old, settled into a very hot, highly thermalized state. All particles except gravitons were in statistical equilibrium at a common, declining temperature, until the dark matter and the neutrinos dropped out of equilibrium and (like the gravitons) became thermodynamically isolated.

During this early relativistic era, the equations of relativistic cosmology imply (as discussed in Sec. 28.4.1) that the temperature *T* of the universe at age *t* satisfied $T/T_P \sim (t/t_P)^{-1/2}$. Here $T_P \equiv [\hbar c^5/(Gk_B^2)]^{1/2} \sim 10^{32}$ K is the Planck temperature, and $t_P \equiv (\hbar G/c^5)^{1/2} \sim 10^{-43}$ s is the Planck time. (This approximate T/T_P relationship can be justified on dimensional grounds.) Now the region that was in causal contact at time *t* (i.e., that was contained within a mutual cosmological horizon) had a volume $\sim (ct)^3$, and thermodynamic considerations imply that the number of relativistic particles that were in causal contact at time *t* was $N \sim (k_B T t/\hbar)^3 \sim (t/t_P)^{3/2}$. (This remains roughly true today when *N* has grown to $\sim 10^{91}$, essentially all in microwave background photons.) The associated entropy was then $S \sim Nk_B$ (cf. Sec. 4.8).

Although this seems like an enormous entropy, gravity can do even better. The most efficient way to create entropy, as described in Sec. 4.10.2, is to form massive black holes. Suppose that out of all the relativistic particle mass within the horizon, $M \sim Nk_BT/c^2$, a fraction f has collapsed into black holes of mass M_H . Then, with the aid of Sec. 4.10.2, we estimate that the associated entropy is $S_H \sim f(M_H/M)(t/t_P)^{1/2}S$. If we use the observation that every galaxy has a central black hole with mass in the $\sim 10^6 - 10^9$ solar mass range, we find that $f \sim 10^{-4}$ and $S_H \sim 10^{11}S$ today!

Now it might be claimed that massive black holes are thermodynamically isolated from the rest of the universe because they will take so long to evaporate. That may be so as a practical matter, but more modest gravitational condensations that create stars and starlight can produce large local departures from thermodynamic equilibrium, accompanied by (indeed, driven by) a net increase of entropy and can produce the conditions necessary for life to develop.





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4.10.4 Structure Formation in the Expanding Universe: Violent Relaxation and Phase Mixing 12

The formation of stars and galaxies ("structure") by gravitational condensation provides a nice illustration of the phase mixing and coarse-graining that underlie the second law of thermodynamics (Sec. 4.7.2).

It is believed that galaxies formed when slight overdensities in the dark matter and gas (presumably irregular in shape) stopped expanding and began to contract under their mutual gravitational attraction. Much of the gas was quickly converted into stars. The dark-matter particles and the stars had very little random motion at this stage relative to their random motions today, $v \sim 200 \text{ km s}^{-1}$. Correspondingly, although their physical volume \mathcal{V}_x was initially only moderately larger than today, their momentum-space volume \mathcal{V}_p was far smaller than it is today. Translated into the language of an ensemble of N such galaxies, the initial coordinate-space volume $\int d^{3N}x \sim \mathcal{V}_x^N$ occupied by each of the ensemble's galaxies was moderately larger than it is today, while its momentum-space volume $\int d^{3N}p \sim V_p^{-N}$ was far smaller. The phase-space volume $\mathcal{V}_x^N \mathcal{V}_p^N$ must therefore have increased considerably during the galaxy formation-with the increase due to a big increase in the relative momenta of neighboring stars. For this to occur, it was necessary that the stars changed their relative energies during the contraction, which requires a time-dependent hamiltonian. In other words, the gravitational potential Φ felt by the stars must have varied rapidly, so that the individual stellar energies would vary according to

$$\frac{dE}{dt} = \frac{\partial H}{\partial t} = m \frac{\partial \Phi}{\partial t}.$$
(4.66)

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The largest changes of energy occurred when the galaxy was contracting dynamically (collapsing), so the potential changed significantly on the timescale it took stars to cross the galaxy, $\tau_{int} \sim 2R/v$. Numerical simulations show that this energy transfer was highly efficient. This process is known as *violent relaxation*. Although violent relaxation could create the observed stellar distribution functions, it was not by itself a means of diluting the phase-space density, since Liouville's theorem still applied.

The mechanism that changed the phase-space density was phase mixing and coarse-graining (Sec. 4.7.2 above). During the initial collapse, the particles and newly formed stars could be thought of as following highly perturbed radial orbits. The orbits of nearby stars were somewhat similar, though not identical. Therefore small elements of occupied phase space became highly contorted as the particles and stars moved along their phase-space paths.

Let us make a simple model of this process by assuming the individual particles and stars initially populate a fraction $f \ll 1$ of the final occupied phase-space volume V_{final} . After one dynamical timescale $\tau_{int} \sim R/v$, this small volume $f V_{\text{final}}$ is (presumably) deformed into a convoluted surface that folds back on itself once or twice like dough being kneaded by a baker, while still occupying the same volume $f V_{\text{final}}$. After *n* dynamical timescales, there are $\sim 2^n$ such folds (cf. Fig. 4.2b above). After $n \sim -\log_2 f$ dynamical timescales, the spacing between folds becomes comparable with the characteristic thickness of this convoluted surface, and it is no longer practical to distinguish the original distribution function. We expect that coarse-graining has been accomplished for all practical purposes; only a pathological physicist would resist it and insist on trying to continue keeping track of which contorted phase-space regions have the original high density and which do not. For a galaxy we might expect that $f \sim 10^{-3}$ and so this natural coarse-graining can occur in a time approximately equal to $-\log_2 10^{-3} \tau_{int} \sim 10 \ \tau_{int} \sim 10^9$ yr, which is 10 times shorter than the present age of galaxies. Therefore it need not be a surprise that the galaxy we know best, our own Milky Way, exhibits little obvious vestigial trace of its initial high-density (low phase-space-volume) distribution function.20

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6 is {101}, 7 is {110}, 8 is {111}, etc.). If $N_{\text{states}} = 4$, then the number of binary digits needed is 2 (the leading 0 in the enumeration above can be dropped), so in measuring the system's state we gain 2 bits of information. If $N_{\text{states}} = 8$, the number of binary digits needed is 3, so our measurement gives us 3 bits of information. In general, we need $\log_2 N_{\text{states}}$ binary digits to distinguish the states from one another, so the amount of information gained in measuring the system's state is the base-2 logarithm of the number of states the system could have been in:

$$I = \log_2 N_{\text{states}} = (1/\ln 2) \ln N_{\text{states}} = 1.4427 \ln N_{\text{states.}}$$
(4.67a)

Notice that this information gain is proportional to the entropy $S = k_B \ln N_{\text{states}}$ of the system before the measurement was made:

$$I = S/(k_B \ln 2).$$
 (4.67b)

The measurement reduces the system's entropy from $S = k_B \ln N_{\text{states}}$ to zero (and increases the entropy of the rest of the universe by at least this amount), and it gives us $I = S/(k_B \ln 2)$ bits of information about the system. We shall discover below that this entropy/information relationship is true of measurements made on a system drawn from any ensemble, not just a microcanonical ensemble. But first we must develop a more complete understanding of information.

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If there are only two possible symbols, we have one bit per symbol in our message. If there are four possible (equally likely) symbols, we have two bits per symbol, and so forth.

It is usually the case that not all symbols occur with the same frequency in the allowed messages. For example, in English messages the letter "A" occurs with a frequency $p_A \simeq 0.07$, while the letter "Z" occurs with the much smaller frequency $p_Z \simeq 0.001$. All English messages, of character length $L \gg N = 27$, constructed by a typical English speaker, will have these frequencies of occurrence for "A" and "Z". Any purported message with frequencies for "A" and "Z" differing substantially from 0.07 and 0.001 will not be real English messages, and thus need not be included in the binary encoding of messages. As a result, it turns out that the most efficient binary encoding of English messages (the most *compressed* encoding) will use an average number of bits per character somewhat less than $\log_2 N = \log_2 27 = 4.755$. In other words, the average information per character in English language messages is somewhat less than $\log_2 27$.

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A straightforward generalization of this argument (Ex. 4.17) shows that, when one constructs messages with very large length $L \gg N$ from a pool of N symbols that occur with frequencies p_1, p_2, \ldots, p_N , the minimum number of bits required to distinguish all the allowed messages from one another (i.e., the amount of information in each message) is

$$I = L \sum_{n=1}^{N} -p_n \log_2 p_n;$$
(4.70)

so the average information per symbol in the message is

$$\bar{I} = \sum_{n=1}^{N} -p_n \log_2 p_n = (1/\ln 2) \sum_{n=1}^{N} -p_n \ln p_n.$$
(4.71)

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MEMORY AND ENTROPY

Information is also a key concept in the theory of computation. As an important example of the relationship of information to entropy, we cite Landauer's (1961, 1991) theorem: In a computer, when one erases *L* bits of information from memory, one necessarily increases the entropy of the memory and its environment by at least $\Delta S = Lk_B \ln 2$ and correspondingly, one increases the thermal energy (heat) of the memory and environment by at least $\Delta Q = T \Delta S = Lk_B T \ln 2$ (Ex. 4.21).

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Bibliographic Note

Statistical mechanics has inspired a variety of readable and innovative texts. The classic treatment is Tolman (1938). Classic elementary texts are Kittel (2004) and Kittel and Kroemer (1980). Among more modern approaches that deal in much greater depth with the topics covered in this chapter are Lifshitz and Pitaevskii (1980), Chandler (1987), Sethna (2006), Kardar (2007), Reif (2008), Reichl (2009), and Pathria and Beale (2011). The Landau-Lifshitz textbooks (including Lifshitz and Pitaevskii, 1980) are generally excellent after one has already learned the subject at a more elementary level. A highly individual and advanced treatment, emphasizing quantum statistical mechanics, is Feynman (1972). A particularly readable account in which statistical mechanics is used heavily to describe the properties of solids, liquids, and gases is Goodstein (2002). Readable, elementary introductions to information theory are Raisbeck (1963) and Pierce (2012); an advanced text is McEliece (2002).

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Random Processes

These motions were such as to satisfy me, after frequently repeated observation, that they arose neither from currents in the fluid, nor from its gradual evaporation, but belonged to the particle itself.

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RANDOM VARIABLE

A (1-dimensional) *random variable* is a (scalar) function y(t), where t is usually time, for which the future evolution is not determined uniquely by any set of initial data or at least by any set that is knowable to you and me. In other words, *random variable* is just a fancy phrase that means "unpredictable function." Throughout this chapter, we insist for simplicity that our random variables y take on a continuum of *real* values ranging over some interval, often but not always $-\infty$ to $+\infty$. The generalizations to y with complex or discrete (e.g., integer) values, and to independent variables other than time, are straightforward.

Examples of random variables are: (i) the total energy E(t) in a cell of gas that is in contact with a heat bath; (ii) the temperature T(t) at the corner of Main Street and Center Street in Logan, Utah; (iii) the price per share of Google stock P(t); (iv) the mass-flow rate $\dot{M}(t)$ from the Amazon River into the Atlantic Ocean. One can also deal with random variables that are vector or tensor functions of time; in Track-Two portions of this chapter we do so.

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From the probability distributions, we can compute ensemble averages (denoted by brackets). For example, the quantities

$$\langle y(t_1) \rangle \equiv \int y_1 p_1(y_1, t_1) dy_1 \text{ and } \sigma_y^2(t_1) \equiv \left\langle \left[y(t_1) - \langle y(t_1) \rangle \right]^2 \right\rangle$$
 (6.2a)

are the ensemble-averaged value of y and the variance of y at time t_1 . Similarly,

$$\langle y(t_2)y(t_1)\rangle \equiv \int y_2 y_1 p_2(y_2, t_2; y_1, t_1) dy_2 dy_1$$
 (6.2b)

is the average value of the product $y(t_2)y(t_1)$.

CONDITIONAL PROBABILITIES

Besides the (absolute) probability distributions p_n , we also find useful an infinite series of *conditional* probability distributions P_2 , P_3 , ..., defined as

$$P_n(y_n, t_n | y_{n-1}, t_{n-1}; \dots; y_1, t_1) dy_n.$$
(6.3)

This distribution is the probability that, *if* y(t) took on the values $y_1, y_2, \ldots, y_{n-1}$ at times $t_1, t_2, \ldots, t_{n-1}$, then it will take on a value between y_n and $y_n + dy_n$ at a later time t_n .

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Henceforth, throughout this chapter, we restrict attention to random processes that are stationary (at least on the timescales of interest to us); and, accordingly, we use

$$p_1(y) \equiv p_1(y, t_1)$$
 (6.6a)

for the probability, since it does not depend on the time t_1 . We also denote by

$$P_2(y_2, t|y_1) \equiv P_2(y_2, t|y_1, 0) \tag{6.6b}$$

the probability that, if a (realization of a) random process begins with the value y_1 , then after the lapse of time *t* it has the value y_2 .

Ergodic hypothesis

6.2.3 Ergodic Hypothesis

A (stationary) random process (ensemble \mathcal{E} of random variables) is said to satisfy the *ergodic hypothesis* (or, for brevity, it will be called *ergodic*) if and only if it has the following property.

Let y(t) be a random variable in the ensemble \mathcal{E} (i.e., let y(t) be any realization of the process). Construct from y(t) a new ensemble \mathcal{E}' whose members are

$$Y^{K}(t) \equiv y(t + KT), \tag{6.7}$$

where *K* runs over all integers, negative and positive, and where *T* is some very large time interval. Then \mathcal{E}' has the same probability distributions p_n as \mathcal{E} ; that is, $p_n(Y_n, t_n; \ldots; Y_1, t_1)$ has the same functional form as $p_n(y_n, t_n; \ldots; y_1, t_1)$ for all times such that $|t_i - t_j| < T$.

This is essentially the same ergodic hypothesis as we met in Sec. 4.6.

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Ergodic processes

As in Sec. 4.6, because of the ergodic hypothesis, time averages defined using any realization y(t) of a random process are equal to ensemble averages:

$$\bar{F} \equiv \lim_{T \to \infty} \frac{1}{T} \int_{-T/2}^{T/2} F(y(t)) dt = \langle F(y) \rangle \equiv \int F(y) p_1(y) dy, \qquad (6.8)$$

for any function F = F(y). In this sense, each realization of the random process is representative, when viewed over sufficiently long times, of the statistical properties of the process's entire ensemble—and conversely. Correspondingly, we can blur the distinction between the random process and specific realizations of it—and we often do so.

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6.3.1 Markov Processes; Random Walk

A random process y(t) is said to be *Markov* (also sometimes called "Markovian") if and only if all of its future probabilities are determined by its most recently known value:

$$P_n(y_n, t_n | y_{n-1}, t_{n-1}; \dots; y_1, t_1) = P_2(y_n, t_n | y_{n-1}, t_{n-1}) \quad \text{for all } t_n \ge \dots \ge t_2 \ge t_1.$$
(6.9)

This relation guarantees that any Markov process (which, of course, we require to be stationary without saying so) is completely characterized by the probabilities

$$p_1(y) \text{ and } P_2(y_2, t|y_1) \equiv \frac{p_2(y_2, t; y_1, 0)}{p_1(y_1)}$$
 (6.10)

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An example of a Markov process is the *x* component of velocity $v_x(t)$ of a dust particle in an arbitrarily large room,¹ filled with constant-temperature air. Why? Because the molecule's equation of motion is² $mdv_x/dt = F'_x(t)$, and the force $F'_x(t)$ is due to random buffeting by other molecules that are uncorrelated (the kick now is unrelated to earlier kicks); thus, there is no way for the value of v_x in the future to be influenced by any earlier values of v_x except the most recent one.

By contrast, the position x(t) of the particle is not Markov, because the probabilities of future values of x depend not just on the initial value of x, but also on the initial velocity v_x —or, equivalently, the probabilities depend on the values of x at two initial, closely spaced times. The pair $\{x(t), v_x(t)\}$ is a 2-dimensional Markov process (see Ex. 6.23).

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State Space	Type of Parameter		
	Discrete	Continuous	
Discrete	(Discrete-parameter)	Continuous-parameter	
	Markov chain	Markov chain	
Continuous	Discrete-parameter	Continuous-parameter	
	Markov process	Markov process	



THE SMOLUCHOWSKI EQUATION

Choose three (arbitrary) times t_1 , t_2 , and t_3 that are ordered, so $t_1 < t_2 < t_3$. Consider a (realization of an) arbitrary random process that begins with a known value y_1 at t_1 , and ask for the probability $P_2(y_3, t_3|y_1)$ (per unit y_3) that it will be at y_3 at time t_3 . Since the realization must go through some value y_2 at the intermediate time t_2 (though we don't care what that value is), it must be possible to write the probability to reach y_3 as

$$P_2(y_3, t_3|y_1, t_1) = \int P_3(y_3, t_3|y_2, t_2; y_1, t_1) P_2(y_2, t_2|y_1, t_1) dy_2,$$

where the integration is over all allowed values of y_2 . This is not a terribly interesting relation. Much more interesting is its specialization to the case of a Markov process. In that case $P_3(y_3, t_3|y_2, t_2; y_1, t_1)$ can be replaced by $P_2(y_3, t_3|y_2, t_2) = P_2(y_3, t_3 - t_2|y_2, 0) \equiv P_2(y_3, t_3 - t_2|y_2)$, and the result is an integral equation involving only P_2 . Because of stationarity, it is adequate to write that equation for the case $t_1 = 0$:

$$P_2(y_3, t_3|y_1) = \int P_2(y_3, t_3 - t_2|y_2) P_2(y_2, t_2|y_1) dy_2.$$
(6.11)

This is the *Smoluchowski equation* (also called *Chapman-Kolmogorov equation*). It is valid for any Markov random process and for times $0 < t_2 < t_3$. We shall discover its power in our derivation of the Fokker-Planck equation in Sec. 6.9.1.



Indola				
loueis				
	DRY ACTIVE PARTICLE	MODELS FOR A	SINGLE PARTICLE	
Mode	Equations of motion	Parameters	Natural units	
ARD	$\dot{\vec{\mathfrak{r}}}(t)=\vec{p}(t)+\mathrm{Pe}^{-1}\vec{\xi}(t)$	$Pe = -\frac{v_0}{2}$	Time scale: $\tau_{\rm p} = D_{\rm R}^{-1}$	
ADI	$\dot{\phi}(t) = \sqrt{2}\eta(t)$	$\sqrt{2DD_{R}}$	Length scale: $l = l_{\rm p} = v_0 D_{\rm R}^{-1}$	
BTP	$\dot{\vec{\mathfrak{r}}}(\mathfrak{t}) = \vec{p}(\mathfrak{t})$	None ^a	Time scale: $\tau_{\rm p} = \lambda_{\rm t}^{-1}$	
1011	$\dot{\phi}(\mathfrak{t})=\sum_{n}\Delta\phi_{n}\delta(\mathfrak{t}-\tilde{T}_{n})$		Length scale: $l=l_{\rm p}=v_0\lambda_{\rm t}^{-1}$	
AOUP	$\dot{\vec{\mathfrak{r}}}(\mathfrak{t})=\vec{\mathfrak{v}}_0(\mathfrak{t})$	None	Time scale: $\tau_{\rm p}$	
AOOI	$\dot{\vec{\mathfrak{v}}}_0(\mathfrak{t})=-\vec{\mathfrak{v}}_0(\mathfrak{t})+\sqrt{2}\vec{\xi}(\mathfrak{t})$	Hone	Length scale: $l = \sqrt{D\tau_{\rm p}}$	
CAP	$\dot{\vec{\mathbf{t}}}(t) = \vec{p}(t) + \mathrm{Pe}^{-1}\vec{\xi}(t)$	$Pe = \frac{v_0}{\sqrt{2DD_R}}$	Time scale: $\tau_{\rm p} = D_{\rm R}^{-1}$	
OAI	$\dot{\phi}(t) = \tilde{\omega} + \sqrt{2}\eta(t)$	$\tilde{\omega} = \omega \tau_p$	Length scale: $l = l_{\rm p} = v_0 D_{\rm p}^{-1}$	



GAUSSIAN PROCESSES

A random process is said to be Gaussian if and only if all of its (absolute) probability distributions are Gaussian (i.e., have the following form):

$$p_n(y_n, t_n; \dots; y_2, t_2; y_1, t_1) = A \exp\left[-\sum_{j=1}^n \sum_{k=1}^n \alpha_{jk}(y_j - \bar{y})(y_k - \bar{y})\right], \quad (6.14a)$$

where (i) *A* and α_{jk} depend only on the time differences $t_2 - t_1, t_3 - t_1, \ldots, t_n - t_1$; (ii) *A* is a positive normalization constant; (iii) $[\alpha_{jk}]$ is a *positive-definite*, symmetric matrix (otherwise p_n would not be normalizable); and (iv) \bar{y} is a constant, which one readily can show is equal to the ensemble average of *y*,

$$\bar{y} \equiv \langle y \rangle = \int y p_1(y) \, dy.$$
 (6.14b)

Since the conditional probabilities are all computable as ratios of absolute probabilities [Eq. (6.4)], the conditional probabilities of a Gaussian process will be Gaussian.

Gaussian random processes are very common in physics. For example, the total number of particles N(t) in a gas cell that is in statistical equilibrium with a heat bath is a Gaussian random process (Ex. 5.11d); and the primordial fluctuations that gave rise to structure in our universe appear to have been Gaussian (Sec. 28.5.3). In fact, as we saw in Sec. 5.6, macroscopic variables that characterize huge systems in statistical equilibrium always have Gaussian probability distributions. The underlying reason is that, when a random process is driven by a large number of statistically independent, random influences, its probability distributions become Gaussian. This general fact is a consequence of the central limit theorem of probability. We state and prove a simple variant of this theorem.









6.4.1 Correlation Functions;

Let y(t) be a (realization of a) random process with time average \bar{y} . Then the correlation function of y(t) is defined by

$$C_{y}(\tau) \equiv \overline{[y(t) - \bar{y}][y(t + \tau) - \bar{y}]} \equiv \lim_{T \to \infty} \frac{1}{T} \int_{-T/2}^{+T/2} [y(t) - \bar{y}][y(t + \tau) - \bar{y}] dt.$$
(6.19)

This quantity, as its name suggests, is a measure of the extent to which the values of y at times t and t + τ tend to be correlated. The quantity τ is sometimes called the *delay time*, and by convention it is taken to be positive. [One can easily see that, if one also defines $C_y(\tau)$ for negative delay times τ by Eq. (6.19), then $C_y(-\tau) = C_y(\tau)$. Thus nothing is lost by restricting attention to positive delay times.]

As an example, for a Gaussian-Markov process with P_2 given by Doob's formula (6.18a) (Fig. 6.4), we can compute $C(\tau)$ by replacing the time average in Eq. (6.19) with an ensemble average: $C_y(\tau) = \int y_2 y_1 p_2(y_2, \tau; y_1) dy_1 dy_2$. If we use $p_2(y_2, \tau; y_1) = P_2(y_2, \tau; y_1) p_1(y_1)$ [Eq. (6.10)], insert P_2 and p_1 from Eqs. (6.18), and perform the integrals, we obtain

$$C_{y}(\tau) = \sigma_{y}^{2} e^{-\tau/\tau_{r}}.$$
 (6.20)

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6.4.2 Spectral Densities

There are several different normalization conventions for Fourier transforms. In this chapter, we adopt a normalization that is commonly (though not always) used in the theory of random processes and that differs from the one common in quantum theory. Specifically, instead of using the angular frequency ω , we use the ordinary frequency $f \equiv \omega/(2\pi)$. We define the Fourier transform of a function y(t) and its inverse by

$$\tilde{y}(f) \equiv \int_{-\infty}^{+\infty} y(t)e^{i2\pi ft}dt, \qquad y(t) \equiv \int_{-\infty}^{+\infty} \tilde{y}(f)e^{-i2\pi ft}df.$$
(6.23)

Notice that with this set of conventions, there are no factors of $1/(2\pi)$ or $1/\sqrt{2\pi}$ multiplying the integrals. Those factors have been absorbed into the *df* of Eq. (6.23), since $df = d\omega/(2\pi)$.

The integrals in Eq. (6.23) are not well defined as written because a random process y(t) is generally presumed to go on forever so its Fourier transform $\tilde{y}(f)$ is divergent. One gets around this problem by crude trickery. From y(t) construct, by truncation, the function

$$y_T(t) \equiv \begin{cases} y(t) & \text{if } -T/2 < t < +T/2, \\ 0 & \text{otherwise.} \end{cases}$$
(6.24a)

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Then the Fourier transform $\tilde{y}_T(f)$ is finite, and by Parseval's theorem (e.g., Arfken, Weber, and Harris, 2013) it satisfies

$$\int_{-T/2}^{+T/2} [y(t)]^2 dt = \int_{-\infty}^{+\infty} [y_T(t)]^2 dt = \int_{-\infty}^{+\infty} |\tilde{y}_T(f)|^2 df = 2 \int_0^{\infty} |\tilde{y}_T(f)|^2 df.$$
(6.24b)

In the last equality we have used the fact that because $y_T(t)$ is real, $\tilde{y}_T^*(f) = \tilde{y}_T(-f)$, where * denotes complex conjugation. Consequently, the integral from $-\infty$ to 0 of $|\tilde{y}_T(f)|^2$ is the same as the integral from 0 to $+\infty$. Now, the quantities on the two sides of (6.24b) diverge in the limit as $T \to \infty$, and it is obvious from the left-hand side that they diverge linearly as T. Correspondingly, the limit

$$\lim_{T \to \infty} \frac{1}{T} \int_{-T/2}^{+T/2} [y(t)]^2 dt = \lim_{T \to \infty} \frac{2}{T} \int_0^\infty |\tilde{y}_T(f)|^2 df$$
(6.24c)

is convergent.

These considerations motivate the following definition of the *spectral density* (also sometimes called the *power spectrum*) $S_y(f)$ of the random process y(t):

$$S_{y}(f) \equiv \lim_{T \to \infty} \left| \frac{2}{T} \right| \int_{-T/2}^{+T/2} [y(t) - \bar{y}] e^{i2\pi f t} dt \right|^{2}.$$
 (6.25)

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Notice that the quantity inside the absolute value sign is just $\bar{y}_T(f)$, but with the mean of y removed before computation of the Fourier transform. (The mean is removed to avoid an uninteresting delta function in $S_y(f)$ at zero frequency.) Correspondingly, by virtue of our motivating result (6.24c), the spectral density satisfies $\int_0^\infty S_y(f)df = \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{+T/2} [y(t) - \bar{y}]^2 dt = (y - \bar{y})^2 = \sigma_y^2$, or

$$\int_{0}^{\infty} S_{y}(f) df = C_{y}(0) = \sigma_{y}^{2}.$$
(6.26)

Thus the integral of the spectral density of *y* over all positive frequencies is equal to the variance of *y*.

By convention, our spectral density is defined only for nonnegative frequencies f. This is because, were we to define it also for negative frequencies, the fact that y(t) is real would imply that $S_y(f) = S_y(-f)$, so the negative frequencies contain no new information. Our insistence that f be positive goes hand in hand with the factor 2 in the 2/T of definition (6.25): that factor 2 folds the negative-frequency part onto the positive-frequency part. This choice of convention is called the *single-sided spectral density*. Sometimes one encounters a *double-sided spectral density*,

$$S_{y}^{\text{double-sided}}(f) = \frac{1}{2}S_{y}(|f|), \qquad (6.27)$$

in which f is regarded as both positive and negative, and frequency integrals generally run from $-\infty$ to $+\infty$ instead of 0 to ∞ (see, e.g., Ex. 6.7).

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Meaning of the spectral density We can infer the physical meaning of the spectral density from previous experience with light spectra. Specifically, consider the scalar electric field⁶ E(t) of a plane-Нδ Hγ polarized light wave entering a telescope from a distant star, galaxy, or nebula. (We H£ must multiply this E(t) by the polarization vector to get the vectorial electric field.) This E(t) is a superposition of emission from an enormous number of atoms, molecules, and high-energy particles in the source, so it is a Gaussian random process. It is not hard to convince oneself that E(t)'s spectral density $S_E(f)$ is proportional frequency f to the light power per unit frequency $d\mathcal{E}/dtdf$ (the light's power spectrum) entering the telescope. When we send the light through a diffraction grating, we get FIGURE 6.6 A spectrum obtained by sending light through a diffraction grating. The intensity of the this power spectrum spread out as a function of frequency f in the form of specimage is proportional to $d\mathcal{E}/dtdf$, which, in turn, is proportional to the spectral density $S_E(f)$ of the electric field E(t) of the light that entered the diffraction grating. tral lines superposed on a continuum, as in Fig. 6.6. The amount of light power in this spectrum, in some narrow bandwidth Δf centered on some frequency f, is $(d\mathcal{E}/dtdf)\Delta f\propto S_E(f)\Delta f$ (assuming S_E is nearly constant over that band). 182



6.4.4 The Wiener-Khintchine Theorem;

The Wiener-Khintchine theorem says that, for any random process y(t), the correlation function $C_y(\tau)$ and the spectral density $S_y(f)$ are the cosine transforms of each other and thus contain precisely the same information:

$$C_{y}(\tau) = \int_{0}^{\infty} S_{y}(f) \cos(2\pi f \tau) df, \qquad S_{y}(f) = 4 \int_{0}^{\infty} C_{y}(\tau) \cos(2\pi f \tau) d\tau.$$

(6.29)

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The factor 4 results from our folding negative frequencies into positive in our definition of the spectral density.

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Proof of Wiener-Khintchine Theorem. This theorem is readily proved as a consequence of Parseval's theorem: Assume, from the outset, that the mean has been subtracted from y(t), so $\bar{y} = 0$. (This is not really a restriction on the proof, since C_y and S_y are insensitive to the mean of y.) Denote by $y_T(t)$ the truncated y of Eq. (6.24a) and by $\tilde{y}_T(f)$ its Fourier transform. Then the generalization of Parseval's theorem⁷

$$\int_{-\infty}^{+\infty} (gh^* + hg^*) dt = \int_{-\infty}^{+\infty} (\tilde{g}\tilde{h}^* + \tilde{h}\tilde{g}^*) df$$
(6.30a)

[with $g = y_T(t)$ and $h = y_T(t + \tau)$ both real and with $\tilde{g} = \tilde{y}_T(f)$, $\tilde{h} = \tilde{y}_T(f)e^{-i2\pi f\tau}$], states

$$\int_{-\infty}^{+\infty} y_T(t) y_T(t+\tau) dt = \int_{-\infty}^{+\infty} \tilde{y}_T^*(f) \tilde{y}_T(f) e^{-i2\pi f\tau} df.$$
(6.30b)

By dividing by *T*, taking the limit as $T \to \infty$, and using Eqs. (6.19) and (6.25), we obtain the first equality of Eqs. (6.29). The second follows from the first by Fourier inversion.

As an application of the Wiener-Khintchine theorem, we can deduce the spectral density $S_y(f)$ for any Gaussian-Markov process by performing the cosine transform of its correlation function $C_y(\tau) = \sigma_y^2 e^{-\tau/\tau_r}$ [Eq. (6.20)]. The result is $S_y(f) = \frac{(4/\tau_r)\sigma_y^2}{(2\pi f)^2 + (1/\tau_r)^2};$ (6.32)

see Fig. 6.8.



FIGURE 6.8 (a) The correlation function (6.20) and (b) the spectral density (6.32) for a Gaussian-Markov process. The conditional probability $P_2(y_2, \tau | y_1)$ for this process is shown in Fig. 6.4.

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6.6 Noise and Its Types of Spectra

Experimental physicists and engineers encounter random processes in the form of noise that is superposed on signals they are trying to measure. Examples include:

- 1. In radio communication, static on the radio is noise.
- 2. When modulated laser light is used for optical communication, random fluctuations in the arrival times of photons always contaminate the signal; the effects of such fluctuations are called "shot noise" and will be studied in Sec. 6.6.1.
- 3. Even the best of atomic clocks fail to tick with absolutely constant angular frequencies *ω*. Their frequencies fluctuate ever so slightly relative to an ideal clock, and those fluctuations can be regarded as noise.

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Flicker noise

Flicker noise, $S_y \propto 1/f$, gets its name from the fact that, when one looks at the time evolution y(t) of a random process with a flicker-noise spectrum, one sees fluctuations ("flickering") on all timescales, and the rms amplitude of flickering is independent of the timescale one chooses. Stated more precisely, choose any timescale Δt and then choose a frequency $f \sim 3/\Delta t$, so one can fit roughly three periods of oscillation into the chosen timescale. Then the rms amplitude of the fluctuations observed will be $\sqrt{S_y(f)f/3}$, which is a constant independent of f when the spectrum is that of flicker noise, $S_y \propto 1/f$. In other words, flicker noise has the same amount of power in each octave of frequency. Figure 6.10 is an illustration: both graphs shown there depict random processes with flicker-noise spectra. (The differences between the two graphs will be explained in Sec. 6.6.2.) No matter what time interval one chooses, these processes look roughly periodic with one, two, or three oscillations in that time interval; and the amplitudes of those oscillations are independent of the chosen time interval. Flicker noise occurs widely in the real world, at low frequencies, for instance, in many electronic devices, in some atomic clocks, in geophysics (the flow rates of rivers, ocean currents, etc.), in astrophysics (the light curves of quasars, sunspot numbers, etc.); even in classical music. For an interesting discussion, see Press (1978).













Fluctuation-dissipation theorem Friction is generally caused by interaction with the huge number of degrees of freedom of some sort of bath (e.g., the molecules of air against which a moving ball or dust particle pushes). Those degrees of freedom also produce fluctuating forces. In this section, we study the relationship between the friction and the fluctuating forces when the bath is thermalized at some temperature ${\cal T}$ (so it is a heat bath). For simplicity, we restrict ourselves to a specific generalized coordinate \boldsymbol{q} of the system that will interact with a bath (e.g., the x coordinate of the ball or dust particle). We require just one special property for *q*: its time derivative $\dot{q} = dq/dt$ must appear in the system's lagrangian as a kinetic energy, $E_{\text{kinetic}} = \frac{1}{2}m\dot{q}^2,$ (6.70) and in no other way. Here m is a (generalized) mass associated with q. Then the equation of motion for q will have the simple form of Newton's second law, $m\ddot{q} = F$, where F includes contributions ${\mathcal F}$ from the system itself (e.g., a restoring force in the case of a normal mode), plus a force ${\it F}_{\rm bath}$ due to the heat bath (i.e., due to all the degrees of freedom in the bath). This F_{bath} is a random process whose time average is a frictional (damping) force proportional to \dot{q} : $\bar{F}_{\text{bath}} = -R\dot{q}, \quad F_{\text{bath}} \equiv \bar{F}_{\text{bath}} + F'.$ (6.71) Here *R* is the coefficient of friction. The fluctuating part F' of F_{bath} is responsible for driving q toward statistical equilibrium. 194 194



- 1. The system might be a dust particle with q its x coordinate and m its mass. The heat bath might be air molecules at temperature T, which buffet the dust particle, producing Brownian motion.
- 2. The system might be an L-C-R circuit (i.e., an electric circuit containing an inductance L, a capacitance C, and a resistance R) with q the total electric charge on the top plate of the capacitor. The bath in this case would be the many mechanical degrees of freedom in the resistor. For such a circuit, the "equation of motion" is

$$L\ddot{q} + C^{-1}q = F_{\text{bath}}(t) = -R\dot{q} + F',$$
 (6.72)

so the effective mass is the inductance L; the coefficient of friction is the resistance (both denoted R); $-R\dot{q} + F'$ is the total voltage across the resistor; and F' is the fluctuating voltage produced by the resistor's internal degrees of freedom (the bath) and so might better be denoted V'.

3. The system might be the fundamental mode of a 10-kg sapphire crystal with *q* its generalized coordinate (cf. Sec. 4.2.1). The heat bath might be all the other normal modes of vibration of the crystal, with which the fundamental mode interacts weakly.



LANGEVIN EQUATION

In general, the equation of motion for the generalized coordinate q(t) under the joint action of (i) the bath's damping force $-R\dot{q}$, (ii) the bath's fluctuating forces F', and (iii) the system's internal force \mathcal{F} will take the form [cf. Eq. (6.71)]

$$m\ddot{q} + R\dot{q} = \mathcal{F} + F'(t). \tag{6.73}$$

= I_ sin(ot

The internal force \mathcal{F} is derived from the system's hamiltonian or lagrangian in the absence of the heat bath. For the *L*-*C*-*R* circuit of Eq. (6.72) that force is $\mathcal{F} = -C^{-1}q$; for the dust particle, if the particle were endowed with a charge Q and were in an external electric field with potential $\Phi(t, x, y, z)$, it would be $\mathcal{F} = -Q\partial\Phi/\partial x$; for the normal mode of a crystal, it is $\mathcal{F} = -m\omega^2 q$, where ω is the mode's eigenfrequency.

Because the equation of motion (6.73) involves a driving force F'(t) that is a random process, one cannot solve it to obtain q(t). Instead, one must solve it in a statistical way to obtain the evolution of q's probability distributions $p_n(q_1, t_1; \ldots; q_n, t_n)$. This and other evolution equations involving random-process driving terms are called by modern mathematicians *stochastic differential equations*, and there is an extensive body of mathematical formalism for solving them. In statistical physics the specific stochastic differential equation (6.73) is known as the *Langevin equation*.

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ELEMENTARY FLUCTUATION-DISSIPATION THEOREM

Because the damping force $-R\dot{q}$ and the fluctuating force F' both arise from interaction with the same heat bath, there is an intimate connection between them. For example, the stronger the coupling to the bath, the stronger will be the coefficient of friction R and the stronger will be F'. The precise relationship between the dissipation embodied in R and the fluctuations embodied in F' is given by the following *fluctuation-dissipation theorem:* At frequencies

$$f \ll 1/\tau_r, \tag{6.74a}$$

where τ_r is the (very short) relaxation time for the fluctuating force F', the fluctuating force has the spectral density

$$S_{F'}(f) = 4R\left(\frac{1}{2}hf + \frac{hf}{e^{hf/(k_BT)} - 1}\right) \text{ in general,}$$

$$S_{F'}(f) = 4Rk_BT \text{ in the classical domain, } k_BT \gg hf.$$
(6.74c)
(6.74c)

Here T is the temperature of the bath, and h is Planck's constant.

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Notice that in the classical domain, $k_BT \gg hf$, the spectral density has a whitenoise spectrum. In fact, since we are restricting attention to frequencies at which F' has no self-correlations $(f^{-1} \gg \tau_r)$, F' is Markov; and since it is produced by interaction with the huge number of degrees of freedom of the bath, F' is also Gaussian. Thus, in the classical domain F' is a Gaussian-Markov, white-noise process.

At frequencies $f \gg k_B T/h$ (quantum domain), in Eq. (6.74b) the term $S_{F'} = 4R_{\frac{1}{2}}hf$ is associated with vacuum fluctuations of the degrees of freedom that make up the heat bath (one-half quantum of fluctuations per mode as for any quantum mechanical simple harmonic oscillator). In addition, the second term, $S_{F'}(f) = 4Rhf e^{-hf/(k_BT)}$, associated with thermal excitations of the bath's degrees of freedom, is exponentially suppressed because at these high frequencies, the bath's modes have exponentially small probabilities of containing any quanta at all. Since in this quantum domain $S_{F'}(f)$ does not have the standard Gaussian-Markov frequency dependence (6.32), in the quantum domain F' is not a Gaussian-Markov process.

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Proof of the Fluctuation-Dissipation Theorem.

In principle, we can alter the system's internal restoring force \mathcal{F} without altering its interactions with the heat bath [i.e., without altering R or $S_{F'}(f)$]. For simplicity, we set \mathcal{F} to zero so q becomes the coordinate of a free mass. The basic idea of our proof is to choose a frequency f_o at which to evaluate the spectral density of F', and then, in an idealized thought experiment, very weakly couple a harmonic oscillator with eigenfrequency f_o to q. Through that coupling, the oscillator is indirectly damped by the resistance R of q and is indirectly driven by R's associated fluctating force F', which arises from a bath with temperature T. After a long time, the oscillator will reach thermal equilibrium with that bath and will then have the standard thermalized mean kinetic energy ($\bar{E} = k_B T$ in the classical regime). We shall compute that mean energy in terms of $S_{F'}(f_o)$ and thereby deduce $S_{F'}(f_o)$.

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The Langevin equation (6.73) and equation of motion for the coupled free mass and harmonic oscillator are

$$m\ddot{q} + R\dot{q} = -\kappa Q + F'(t), \quad M\ddot{Q} + M\omega_a^2 Q = -\kappa q.$$
 (6.75a)

Here M, Q, and $\omega_o = 2\pi f_o$ are the oscillator's mass, coordinate, and angular eigenfrequency, and κ is the arbitrarily small coupling constant. (The form of the coupling terms $-\kappa Q$ and $-\kappa q$ in the two equations can be deduced from the coupling's interaction hamiltonian $H_I = \kappa q Q$.) Equations (6.75a) can be regarded as a filter to produce from the fluctuating-force input F'(t) a resulting motion of the oscillator, $Q(t) = \int_{-\infty}^{+\infty} K(t - t')F'(t')dt'$. The squared Fourier transform $|\tilde{K}(f)|^2$ of this filter's kernel K(t - t') is readily computed by the standard method [Eq. (6.51) and associated discussion] of inserting a sinusoid $e^{-i\omega t}$ (with $\omega = 2\pi f$) into the filter [i.e., into the differential equations (6.75a)] in place of F', then solving for the sinusoidal output Q, and then setting $|\tilde{K}|^2 = |Q|^2$. The resulting $|\tilde{K}|^2$ is the ratio of the spectral densities of input and output. We carefully manipulate the resulting $|\tilde{K}|^2$ so as to bring it into the following standard resonant form:

$$S_q(f) = |\tilde{K}(f)|^2 S_{F'}(f) = \frac{|B|^2}{(\omega - \omega'_o)^2 + (2M\omega_o^2 R|B|^2)^2]} S_{F'}(f).$$
(6.75b)

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Here $B = \kappa / [2M\omega_o(m\omega_o^2 + iR\omega_o)]$ is arbitrarily small because κ is arbitrarily small; and ${\omega'_o}^2 = \omega_o^2 + 4mM\omega_o^4|B|^2$ is the oscillator's squared angular eigenfrequency after coupling to q, and is arbitrarily close to ω_o^2 because $|B|^2$ is arbitrarily small. In these equations we have replaced ω by ω_o everywhere except in the resonance term $(\omega - \omega'_o)^2$ because $|\tilde{K}|^2$ is negligibly small everywhere except near resonance, $\omega \cong \omega_o$.

The mean energy of the oscillator, averaged over an arbitrarily long timescale, can be computed in either of two ways.

1. Because the oscillator is a mode of some boson field and is in statistical equilibrium with a heat bath, its mean occupation number must have the standard Bose-Einstein value $\eta = 1/[e^{\hbar\omega_o/(k_BT)} - 1]$, and since each quantum carries an energy $\hbar\omega_o$, the mean energy is

$$\bar{E} = \frac{\hbar\omega_o}{e^{\hbar\omega_o/(k_BT)} - 1} + \frac{1}{2}\hbar\omega_o.$$
(6.75c)

Here we have included the half-quantum of energy associated with the mode's vacuum fluctuations.

2. Because on average the energy is half potential and half kinetic, and the mean potential energy is $\frac{1}{2}m\omega_o^2\overline{Q^2}$, and because the ergodic hypothesis tells us that time averages are the same as ensemble averages, it must be that

$$\bar{E} = 2\frac{1}{2}M\omega_o^2\omega^2 \langle Q^2 \rangle = M\omega_o^2 \int_0^\infty S_Q(f) df.$$
 (6.75d)

By inserting the spectral density (6.75b) and performing the frequency integral with the help of the narrowness of the resonance, we obtain

$$\bar{E} = \frac{S_{F'}(f_o)}{4R}.$$
(6.75e)

Equating this to our statistical-equilibrium expression (6.75c) for the mean energy, we see that at the frequency $f_o = \omega_o/(2\pi)$ the spectral density $S_{F'}(f_o)$ has the form (6.74b) claimed in the fluctuation-dissipation theorem. Moreover, since f_o can be chosen to be any frequency in the range (6.74a), the spectral density $S_{F'}(f)$ has the claimed form anywhere in this range.

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BROWNIAN MOTION

In Secs. 6.3.3 and 6.7.2, we have studied the Brownian motion of a dust particle being buffeted by air molecules, but until now we omitted any attempt to deduce the motions relaxation time τ_r . We now apply the fluctuation-dissipation theorem to deduce t_r , using a model in which the particle is idealized as a sphere with mass *m* and radius *a* that, of course, is far larger than the air molecules.

The equation of motion for the dust particle, when we ignore the molecules' fluctuating forces, is mdv/dt = -Rv. Here the resistance (friction) R due to interaction with the molecules has a form that depends on whether the molecules' mean free path λ is small or large compared to the particle. From the kinetic-theory formula $\lambda = 1/(ar_{mol})$, where n is the number density of molecules and σ_{mol} is their cross section to scatter off each other (roughly their cross sectional area), we can deduce that for air $\lambda \sim 0.1 \mu$ m. This is tiny compared to a dust particle's radius $a \sim 10$ to $1,000 \mu$ m. This means that, when interacting with the dust particle, the air molecules will behave like a fluid. As we shall learn in Chap. 15, the friction for a fluid depends on whether a quantity called the Reynolds number, R = va/v, is small or large compared to unity; here $v \sim 10^{-5} m^2 s^{-1}$ is the kinematic viscosity of air. Inserting numbers, we see that $R \sim (v/0.1 m s^{-1})(a/100 \mu$ m). The speeds v of dust particles being buffeted by air are far smaller than 0.1 m s^{-1} as anyone who has watched them in a sunbeam knows, or as you can estimate from Eq. (6.53a). Therefore, the Reynolds number is small. From an analysis carried out in Sec. 14.3.2, we learn that in this low. Re fluid regime, the resistance (friction) on our spherical particle with radius a is [Eq. (14.34)]

$$R = 6\pi\rho va, \tag{6.76}$$

where $\rho \sim 1 \text{ kg m}^{-3}$ is the density of air. (Notice that this resistance is proportional to the sphere's radius *a* or circumference; if λ were $\gg a$, then *R* would be proportional to the sphere's cross sectional area, i.e., to a^2 .)



6.9 Fokker-Planck Equation

In statistical physics, we often want to know the collective influence of many degrees of freedom (a bath) on a single (possibly vectorial) degree of freedom q. The bath might or might not be thermalized. The forces it exerts on q might have short range (as in molecular collisions buffeting an air molecule or dust particle) or long range (as in Coulomb forces from many charged particles in a plasma pushing stochastically on an electron that interests us, or gravitational forces from many stars pulling on a single star of interest). There might also be long-range, macroscopic forces that produce anisotropies and/or inhomogeneities (e.g., applied electric or magnetic fields). We might want to compute how the bath's many degrees of freedom influence, for example, the diffusion of a particle as embodied in its degree of freedom q. Or we might want to compute the statistical properties of q for a representative electron in a plasma and from them deduce the plasma's transport coefficients (diffusivity, heat conductivity, and thermal conductivity). Or we might want to know how the gravitational pulls of many stars in the vicinity of a black hole drive the collective evolution of the stars' distribution function.

6.9.1 Fokker-Planck for a 1-Dimensional Markov Process

For a 1-dimensional Markov process y(t) (e.g., the *x* component of the velocity of a particle) being driven by a bath (not necessarily thermalized!) with many degrees of freedom, the *Fokker-Planck equation*¹¹ states

$$\frac{\partial}{\partial t}P_2 = -\frac{\partial}{\partial y}[A(y)P_2] + \frac{1}{2}\frac{\partial^2}{\partial y^2}[B(y)P_2].$$
(6.94)

Here $P_2 = P_2(y, t|y_o)$ is to be regarded as a function of the variables *y* and *t* with y_o fixed; that is, Eq. (6.94) is to be solved subject to the initial condition

$$P_2(y, 0|y_o) = \delta(y - y_o).$$
(6.95)

As we shall see later, this Fokker-Planck equation is a generalized diffusion equation for the probability P_2 : as time passes, the probability diffuses away from its initial location, $y = y_o$, spreading gradually out over a wide range of values of y.

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In the Fokker-Planck equation (6.94) the function A(y) produces a motion of the mean away from its initial location, while the function B(y) produces a diffusion of the probability. If one can deduce the evolution of P_2 for very short times by some other method [e.g., in the case of a dust particle being buffeted by air molecules, by solving statistically the Langevin equation mdv/dt + Rv = F'(t)], then from that short-time evolution one can compute the functions A(y) and B(y):

$$A(y) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{-\infty}^{+\infty} (y' - y) P_2(y', \Delta t | y) dy',$$
(6.96a)

$$B(y) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{-\infty}^{+\infty} (y' - y)^2 P_2(y', \Delta t | y) dy'.$$
 (6.96b)

(These equations can be deduced by reexpressing the limit as an integral of the time derivative $\partial P_2/\partial t$ and then inserting the Fokker-Planck equation and integrating by parts; Ex. 6.19.) Note that the integral (6.96a) for A(y) is the mean change $\overline{\Delta y}$ in the value of *y* that occurs in time Δt , if at the beginning of Δt (at t = 0) the value of the process is precisely *y*; moreover (since the integral of yP_2 is just equal to *y*, which is a constant), A(y) is also the rate of change of the mean, $d\bar{y}/dt$. Correspondingly we can write Eq. (6.96a) in the more suggestive form

$$A(y) = \lim_{\Delta t \to 0} \left(\frac{\overline{\Delta y}}{\Delta t} \right) = \left(\frac{d\bar{y}}{dt} \right)_{t=0}.$$
 (6.97a)

Similarly, the integral (6.96b) for B(y) is the mean-squared change in y, $\overline{(\Delta y)^2}$, if at the beginning of Δt the value of the process is precisely y; and (as one can fairly easily show; Ex. 6.19) it is also the rate of change of the variance $\sigma_y^2 = \int (y' - \bar{y})^2 P_2 dy'$. Correspondingly, Eq. (6.96b) can be written as

$$B(y) = \lim_{\Delta t \to 0} \left(\frac{\overline{(\Delta y)^2}}{\Delta t} \right) = \left(\frac{d\sigma_y^2}{dt} \right)_{t=0}.$$

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(6.97b)



DERIVATION OF THE FOKKER-PLANCK EQUATION (6.94)

Because *y* is Markov, it satisfies the Smoluchowski equation (6.11), which we rewrite here with a slight change of notation:

$$P_2(y, t+\tau|y_o) = \int_{-\infty}^{+\infty} P_2(y-\xi, t|y_o) P_2(y-\xi+\xi, \tau|y-\xi) d\xi. \quad (6.98a)$$

Take τ to be small so only small ξ will contribute to the integral, and expand in a Taylor series in τ on the left-hand side of (6.98a) and in the ξ of $y - \xi$ on the right-hand side:

$$P_{2}(y,t|y_{o}) + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\frac{\partial^{n}}{\partial t^{n}} P_{2}(y,t|y_{o}) \right] \tau^{n}$$

$$= \int_{-\infty}^{+\infty} P_{2}(y,t|y_{o}) P_{2}(y+\xi,\tau|y) d\xi$$

$$+ \sum_{n=1}^{\infty} \frac{1}{n!} \int_{-\infty}^{+\infty} (-\xi)^{n} \frac{\partial^{n}}{\partial y^{n}} \left[P_{2}(y,t|y_{o}) P_{2}(y+\xi,\tau|y) \right] d\xi. \quad (6.98b)$$

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In the first integral on the right-hand side the first term is independent of ξ and can be pulled out from under the integral, and the second term then integrates to one; thereby the first integral on the right reduces to $P_2(y, t|y_o)$, which cancels the first term on the left. The result is then

$$\sum_{n=1}^{\infty} \frac{1}{n!} \left[\frac{\partial^n}{\partial t^n} P_2(y, t|y_o) \right] \tau^n$$
$$= \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial y^n} \left[P_2(y, t|y_o) \int_{-\infty}^{+\infty} \xi^n P_2(y+\xi, \tau|y) \, d\xi \right].$$
(6.98c)

Divide by $\tau,$ take the limit $\tau \rightarrow 0,$ and set $\xi \equiv y'-y$ to obtain

$$\frac{\partial}{\partial t}P_2(y,t|y_o) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial y^n} [M_n(y)P_2(y,t|y_o)],\tag{6.99a}$$

where

$$M_n(\mathbf{y}) \equiv \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{-\infty}^{+\infty} (\mathbf{y}' - \mathbf{y})^n P_2(\mathbf{y}', \Delta t | \mathbf{y}) \, d\mathbf{y}' \tag{6.99b}$$

is the *n*th moment of the probability distribution P_2 after time Δt . This is a form of the Fokker-Planck equation that has slightly wider validity than Eq. (6.94). Almost always, however, the only nonvanishing functions $M_n(y)$ are $M_1 \equiv A$, which describes the linear motion of the mean, and $M_2 \equiv B$, which describes the linear growth of the variance. Other moments of P_2 grow as higher powers of Δt than the first power, and correspondingly, their M_n s vanish. Thus, almost always¹² (and always, so far as we are concerned), Eq. (6.99a) reduces to the simpler version (6.94) of the Fokker-Planck equation.

TIME-INDEPENDENT FOKKER-PLANCK EQUATION

If, as we assume in this chapter, *y* is ergodic, then $p_1(y)$ can be deduced as the limit of $P_2(y, t|y_o)$ for arbitrarily large times *t*. Then (and in general) p_1 can be deduced from the time-independent Fokker-Planck equation:

$$-\frac{\partial}{\partial y}[A(y)p_1(y)] + \frac{1}{2}\frac{\partial^2}{\partial y^2}[B(y)p_1(y)] = 0.$$
(6.100)

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GAUSSIAN-MARKOV PROCESS

For a Gaussian-Markov process, the mathematical form of $P_2(y_2, t|y_1)$ is known from Doob's theorem: Eqs. (6.18). In the notation of those equations, the Fokker-Planck functions *A* and *B* are

$$A(y_1) = (d\bar{y}_t/dt)_{t=0} = -(y_1 - \bar{y})/\tau_r, \text{ and } B(y_1) = (d\sigma_{y_1}^2/dt)_{t=0} = 2\sigma_y^2/\tau_r.$$

Translating back to the notation of this section, we have

$$A(y) = -(y - \bar{y})/\tau_r, \qquad B(y) = 2\sigma_y^2/\tau_r.$$
 (6.101)

Thus, if we can compute A(y) and B(y) explicitly for a Gaussian-Markov process, then from them we can read off the process's relaxation time τ_r , long-time mean \bar{y} , and long-time variance σ_y^2 . As examples, in Ex. 6.22 we revisit Brownian motion of a dust particle in air and in the next section, we analyze laser cooling of atoms. A rather different example is the evolution of a photon distribution function under Compton scattering (Sec. 28.6.3).

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Bibliographic Note

Random processes are treated in many standard textbooks on statistical physics, typically under the rubric of fluctuations or nonequilibrium statistical mechanics (and sometimes not even using the phrase "random process"). We like Kittel (2004), Sethna (2006), Reif (2008), and Pathria and Beale (2011). A treatise on signal processing that we recommend, despite its age, is Wainstein and Zubakov (1962). There are a number of textbooks on random processes (also called "stochastic processes" in book titles), usually aimed at mathematicians, engineers, or finance folks (who use the theory of random processes to try to make lots of money, and often succeed). But we do not like any of those books as well as the relevant sections in the above statistical mechanics texts. Nevertheless, you might want to peruse Lax et al. (2006), Van Kampen (2007), and Paul and Baschnagel (2010).