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Newtonian trajectories and quantum waves in expanding force fields

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Abstract. We study non-relativistic particles and waves in N dimensions in a time-dependent potential $V(\boldsymbol{r}/l(t))/(l(t))^2$, which describes a force field that expands and weakens as the scale factor l increases. If l^2 is a quadratic function of time, then, in a reference frame expanding with the system and employing clocks recalibrated to read a scaled time that depends on $l(t)$, the classical and quantum evolutions can be described by a conservative Hamiltonian differing from the original one by an 'inertial' term quadratic in the position variables. The quantal 'expanding modes' form a complete set whose energies decrease and which carry current outwards from the centre of expansion. Non-equilibrium statistical ensembles can be constructed, expanding with the force field.

1. Introduction

We shall consider, classically and quantum mechanically, certain non-relativistic systems which depend on a spatial scaling parameter, l. This parameter is assumed to change at a finite rate, and, for these systems, we intend to generalise the theorem concerning adiabatic invariants which, in its familiar form, holds only in the limit of infinitely slow changes (cf e.g. Whittaker 1953 or Arnold 1978). A system is specified by its Hamiltonian function H: let it be that of a particle of mass m moving in a non-conservative potential field V in a space of N dimensions. The linear scale factor $l = l(t)$ governs an isotropic expansion, or contraction, of this field, so that

$$H(\boldsymbol{r}, \boldsymbol{p}, l(t)) = \tfrac{1}{2}p^2/m + \alpha(l(t))V(\boldsymbol{r}/l(t)), \tag{1.1}$$

where the multiplier $\alpha(l)$ scales the strength of the expanding field. Such a Hamiltonian includes the important case of an expanding cavity, for which, at all times, the potential term would vanish inside the cavity and be infinite outside it.

It is a surprising fact that whatever the form of V, the functions $l(t)$ and $\alpha(l)$ can be chosen in such a way that, with appropriate scaling of the time also, the particle can be considered as moving in a conservative field. Relations between the Hamiltonians, and between the Hamilton principal functions, in the original and scaled coordinates are then very simple. A consequence of this is that in the wave-mechanical treatment any quantum state can be expressed as a superposition of expanding modes whose wavefunctions are solutions of time-independent equations of the Schrödinger type. Ensembles of classical trajectories or quantum states can be chosen which are stationary in the expanding reference frame, and this raises the intriguing possibility of an exact statistical-mechanical description for certain processes occurring at finite rate.

2. Classical trajectories

From the Hamiltonian (1.1) it follows that the particle trajectory $\boldsymbol{r} = \boldsymbol{r}(t)$ is determined by Newton's equation of motion,

$$m\, \mathrm{d}^2\boldsymbol{r}/\mathrm{d}t^2 = -\alpha \partial V(\boldsymbol{r}/l)/\partial \boldsymbol{r}. \tag{2.1}$$

With the change of variable

$$\boldsymbol{\rho} \equiv \boldsymbol{r}/l(t), \tag{2.2}$$

and a new time variable $\tau = \tau(t)$, to be defined presently, the equation of motion becomes

$$\frac{ml^2\tau'^2}{\alpha}\frac{\mathrm{d}^2\boldsymbol{\rho}}{\mathrm{d}\tau^2} + \frac{m(l^2\tau')'}{\alpha}\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}\tau} + \frac{mll''}{\alpha}\boldsymbol{\rho} = -\frac{\partial V(\boldsymbol{\rho})}{\partial \boldsymbol{\rho}}, \tag{2.3}$$

where the primes denote differentiation with respect to t. The functions $l(t)$, $\tau(t)$ and $\alpha(l)$ can now be determined so that the motion of the particle, when described in terms of the new variables, appears to take place in a conservative field of force.

In order for the second, 'dissipative', term in (2.3) to vanish, it is necessary that

$$l^2\tau' = \text{constant} \equiv 1, \qquad \text{i.e., } \tau(t) = \int_0^t \frac{\mathrm{d}t}{l^2(t)}, \tag{2.4}$$

where the choice of unity for the constant and of zero for $\tau(0)$ involve no loss of generality. For the first term to reduce to $m\mathrm{d}^2\boldsymbol{\rho}/\mathrm{d}\tau^2$, we then want

$$\alpha = 1/l^2. \tag{2.5}$$

The last term in (2.3) can survive, provided its coefficient is independent of time, which requires

$$ml^3l'' = k, \tag{2.6}$$

where k is constant. This equation has the solution

$$l(t) = (at^2 + 2bt + c)^{1/2}, \tag{2.7}$$

with the coefficients restricted by

$$ac - b^2 = k/m. \tag{2.8}$$

Thus (2.3) simplifies to

$$m\mathrm{d}^2\boldsymbol{\rho}/\mathrm{d}\tau^2 = -\partial(V(\boldsymbol{\rho}) + \tfrac{1}{2}k\rho^2)/\partial\boldsymbol{\rho}. \tag{2.9}$$

This result allows the following physical interpretation. Let measuring rods expand with the system to measure $\boldsymbol{\rho}$ instead of $\boldsymbol{r}$, and let clocks be recalibrated to read τ instead of t. In this frame of reference the particle appears to move in a conservative field consisting of $V(\boldsymbol{\rho})$ plus the central force $-k\boldsymbol{\rho}$ (which is inertial in origin, reflecting the fact that observers in the expanding frame would accelerate). The central force attracts particles to the centre of expansion if $k > 0$, and repels them if $k < 0$.

The class of linear scaling factors $l(t)$ for which (2.7) holds, corresponds precisely to the exceptional expansion rates for which the study of repeated elastic reflections of a particle in an expanding spherical cavity simplifies considerably, as shown elsewhere (Klein and Mulholland 1978). There, the treatment included the more general cases of relativistic motion and of radiation, while here the more general cases of arbitrary potential V and any dimensionality N are investigated.

The fate of trajectories as $t \to \infty$ depends on the convergence of the integral (2.4) for τ. If $a > 0$ in the expansion law (2.7), τ tends to a finite limit, implying a constant terminal velocity $d\boldsymbol{r}/dt$ in the original reference frame. The particle becomes effectively free as the field, where its intensity is appreciable, recedes to infinity with a speed greater than the terminal velocity—in an expanding cavity the particle would be left behind by the receding walls. The same applies to the exceptional case of linear expansion, for which $b^2 = ac$ so that $k = 0$ and there is no inertial force. In the case $a = 0$, $b > 0$, $\tau \to \infty$ as $t \to \infty$, the expansion rate dl/dt decreases and the particle continues to interact with the field at all times.

In cases of contraction, where l vanishes at some time t_0, the situation is different, since for all a and b the integral for τ diverges as $t \to t_0$: as the force field closes in, the particle experiences, in a flash, an eternity of interaction as measured on the τ-scale.

For later reference we note the following identities implied by (2.7) and (2.8)

$$ll'' + l'^2 = a, \qquad \tfrac{1}{2}(l'/l)' = (k/m)/l^4 - \tfrac{1}{2}a/l^2, \qquad (ll')^2 = al^2 - k/m. \qquad (2.10a, b, c)$$

3. Hamiltonian formulation

With (2.5), the Hamiltonian (1.1) becomes

$$H(\boldsymbol{r}, \boldsymbol{p}, l) = \tfrac{1}{2}p^2/m + (1/l^2)V(\boldsymbol{r}/l), \qquad (3.1)$$

and of course this is not conservative because l depends on time. In the expanding frame, however, the equation of motion (2.9) can be generated by the conservative Hamiltonian

$$\mathscr{H}(\boldsymbol{\rho}, \boldsymbol{\pi}; k) = \tfrac{1}{2}\pi^2/m + V(\boldsymbol{\rho}) + \tfrac{1}{2}k\rho^2, \qquad (3.2)$$

where

$$\boldsymbol{\pi} = l\boldsymbol{p} - ml'\boldsymbol{r} \qquad (3.3)$$

is the momentum conjugate to $\boldsymbol{\rho}$. The last relation comes from (2.2) and (2.4) together with Hamilton's equations for H and $\mathscr{H}$. With the aid of (2.10c), $\mathscr{H}$ can be expressed in terms of the original variables:

$$\mathscr{H} = l^2 H - ll'\boldsymbol{r}\cdot\boldsymbol{p} + \tfrac{1}{2}mar^2. \qquad (3.4)$$

The converse relation is

$$H = (\mathscr{H} - k\rho^2)/l^2 + \tfrac{1}{2}ma\rho^2 + (l'/l)\boldsymbol{\rho}\cdot\boldsymbol{\pi}. \qquad (3.5)$$

Now, the numerical value of $\mathscr{H}$ is the constant 'energy' of motion in the $(\boldsymbol{\rho}, \tau)$ reference system, and therefore the function on the right of (3.4) is a constant of the motion along any particular trajectory in the original $(\boldsymbol{r}, t)$ reference system. This function is an invariant of the dynamical system with respect to changes in the parameter l, provided they are in accord with the expansion rule (2.7). Such changes need not be slow, as in the original theorem on adiabatic invariants, but may take place at a finite rate.

The Hamilton–Jacobi equations for H and $\mathscr{H}$ are, respectively,

$$(1/2m)(\partial W/\partial\boldsymbol{r})^2 + (1/l^2)V(\boldsymbol{r}/l) = -\partial W/\partial t \qquad (3.6)$$

and

$$(1/2m)(\partial\mathscr{W}/\partial\boldsymbol{\rho})^2 + V(\boldsymbol{\rho}) + \tfrac{1}{2}k\rho^2 = -\partial\mathscr{W}/\partial\tau, \qquad (3.7)$$

where W is Hamilton's principal function corresponding to H (and depends on $\boldsymbol{r}$ and t) and $\mathscr{W}$ corresponds to $\mathscr{H}$ (and depends on $\boldsymbol{\rho}$ and τ). The relation between corresponding solutions of these equations can be shown, with the aid of (2.4) and (2.6), to be

$$W = \mathscr{W} + \tfrac{1}{2} m l l' \rho^2, \tag{3.8}$$

apart from an arbitrary additive constant.

4. Expanding modes in wavemechanics

The Schrödinger equations obtained from (3.1) and (3.2) for the Hamiltonians H and $\mathscr{H}$ are, respectively,

$$-(\hbar^2/2m)\partial^2\psi/\partial \boldsymbol{r}^2 + (1/l^2)V(\boldsymbol{r}/l)\psi = \mathrm{i}\hbar\partial\psi/\partial t \tag{4.1}$$

and

$$-(\hbar^2/2m)\partial^2\phi/\partial\boldsymbol{\rho}^2 + (V(\boldsymbol{\rho}) + \tfrac{1}{2}k\rho^2)\phi = \mathrm{i}\hbar\partial\phi/\partial\tau. \tag{4.2}$$

By direct substitution one can verify that the solutions of these equations are related by

$$\psi(\boldsymbol{r}, t) = (l(t))^{-N/2}\phi(\boldsymbol{\rho}, \tau)\exp[(\mathrm{i}/2\hbar)mll'\rho^2], \tag{4.3}$$

apart from an arbitrary constant factor.

This relation is already suggested by the connection, (3.8), between the solutions of the Hamilton–Jacobi equations and the phase of the wavefunction (Dirac 1947). It is nevertheless remarkable that the phase of (4.3) is given *exactly* by this connection, which in general gives only a semiclassical approximation. The problem under discussion is thus similar to that of the free particle, the harmonic oscillator, and the Coulomb potential, for which semiclassical methods yield exact results. The presence of the factor $l^{-N/2}$ in (4.3) is also not unexpected: it is a trivial consequence of the expansion, and guarantees that the probability density remains normalised in N-dimensional space.

As $\mathscr{H}$ is independent of τ, it is possible to obtain solutions of (4.2) by separation of variables, in the form

$$\phi(\boldsymbol{\rho}, \tau) = u(\boldsymbol{\rho})\exp(-\mathrm{i}\mathscr{E}\tau/\hbar). \tag{4.4}$$

We shall therefore have eigenfunctions $u_n(\boldsymbol{\rho})$, and corresponding eigenvalues $\mathscr{E}_n$, satisfying

$$-(\hbar^2/2m)\partial^2 u_n/\partial\boldsymbol{\rho}^2 + (V(\boldsymbol{\rho}) + \tfrac{1}{2}k\rho^2)u_n = \mathscr{E}_n u_n, \tag{4.5}$$

together with boundary conditions (which of course must not depend on τ); as is usual in multidimensional separable systems the label n can denote several indices labelling the state. The wavefunction ψ of (4.2), in the original variables, is then a superposition of 'expanding modes':

$$\psi_n(\boldsymbol{r}, t) = (l(t))^{-N/2}\exp[(\mathrm{i}/\hbar)(ml'/2l)r^2 - \mathscr{E}_n\tau(t)]u_n(\boldsymbol{r}/l(t)). \tag{4.6}$$

That is, there are eigenfunctions even in the case of varying potential field. Despite the evolution of the system 'the undulatory content remains similar to itself' (Larmor 1900).

For a system in the nth expanding mode ψ_n, the expectation value of its energy, $E_n(t)$, at time t is the expectation value of the Hamiltonian operator $\hat{H}$ corresponding to (3.1), viz,

$$E_n(t) = \langle\psi_n|\hat{H}|\psi_n\rangle = \left(\int \mathrm{d}^N\boldsymbol{r}\,\psi_n^* \mathrm{i}\hbar\,\partial\psi_n/\partial t\right) \Big/ \left(\int \mathrm{d}^N\boldsymbol{r}|\psi_n|^2\right). \tag{4.7}$$

On substituting from (4.6) and using (2.10*b*) it follows straightforwardly that

$$E_n(t) = (1/l(t))^2(\mathscr{E}_n - k\langle\rho^2\rangle_n) + \tfrac{1}{2}ma\langle\rho^2\rangle_n, \tag{4.8}$$

where

$$\langle\rho^2\rangle_n \equiv \int \mathrm{d}^N\boldsymbol{\rho}\,\rho^2|u_n(\boldsymbol{\rho})|^2 \Big/ \int d^N\boldsymbol{\rho}|u_n(\boldsymbol{\rho})|^2 \tag{4.9}$$

is the constant expectation value of ρ^2 belonging to the nth eigenstate satisfying (4.5). The result (4.8) can also be obtained from (3.5) on replacing $\boldsymbol{\rho}\cdot\boldsymbol{\pi}$ by the Hermitian operator $\frac{1}{2}(\hat{\boldsymbol{\rho}}\cdot\hat{\boldsymbol{\pi}} + \hat{\boldsymbol{\pi}}\cdot\hat{\boldsymbol{\rho}})$, etc.

If the expansion continues forever, (4.8) gives

$$E_n(t) \to \tfrac{1}{2}ma\langle\rho^2\rangle_n \qquad \text{as } t\to\infty. \tag{4.10}$$

This is finite if $a \neq 0$, and $a > 0$ is the case discussed in § 2, where the force field leaves the particles behind, so that the asymptotic state is a wavepacket expanding into empty space. If $a = 0$, however, the particles continually work on the field and $E_n \to 0$ as $t\to\infty$ for all states ψ_n.

The decrease in energy implies a continual local redistribution of the wave, and this is expressed, for the mode ψ_n, by the probability current (expectation value of the Hermitian local velocity operator)

$$\begin{aligned} \boldsymbol{j}_n(\boldsymbol{r}, t) &\equiv \langle\psi_n|\tfrac{1}{2}[(\hat{\boldsymbol{p}}/m)\delta(\hat{\boldsymbol{r}}-\boldsymbol{r}) + \delta(\hat{\boldsymbol{r}}-\boldsymbol{r})\hat{\boldsymbol{p}}/m]|\psi\rangle \\ &= (\hbar/m)\,\mathrm{Im}\,\psi_n^*\,\partial\psi_n/\partial\boldsymbol{r}. \end{aligned} \tag{4.11}$$

From (4.6) one finds

$$\boldsymbol{j}_n(\boldsymbol{r}, t) = |\psi_n(\boldsymbol{r}, t)|^2(l'/l)\boldsymbol{r} = (1/l)^N|u_n(\boldsymbol{r}/l)|^2(l'/l)\boldsymbol{r}. \tag{4.12}$$

Thus $\boldsymbol{j}_n$ is directed radially outwards from the centre of expansion, or inwards if the potential field is contracting.

Expanding modes will exist only if the amplitude functions $u_n(\boldsymbol{\rho})$ exist and correspond to a discrete spectrum of eigenvalues $\mathscr{E}_n$. This spectrum depends on the modified potential $V + \frac{1}{2}k\rho^2$ and on the boundary conditions; one can think of the boundary conditions as geometrical idealisations, as in the case of hard walls, or as included in the field V. The effect of the parabolic term $\frac{1}{2}k\rho^2$ depends on whether the expansion is accelerating or decelerating (cf 2.6), and will be clarified by the consideration of particular cases, to which we now turn.

5. Special cases

5.1. Free particle

The Hamiltonian (1.1) is $H = \frac{1}{2}p^2/m$, and according to Newtonian mechanics the particle will describe a straight line with constant speed in the $(\boldsymbol{r}, t)$ reference frame. It is easily shown from (2.2) and (2.7) that in the non-inertial frame $(\boldsymbol{\rho}, \tau)$ the path appears as a hyperbola if $k<0$ and as an elliptical arc if $k>0$. In the latter case, equation (2.9) is that of an N-dimensional isotropic harmonic oscillator. The motion is conservative in both reference frames and (3.4) is easily verified, with both $\mathscr{H}$ and H as numerical constants and both l^2 and r^2 as quadratic functions of the time.

In the quantum mechanical treatment we have for the case $k>0$ the paradox that in the $(\boldsymbol{r}, t)$ frame there is a continuous energy spectrum for the free particle, while in the $(\boldsymbol{\rho}, \tau)$ frame the 'energy' $\mathscr{E}$ has the discrete spectrum of a N-dimensional harmonic oscillator. Now, the wavefunctions (4.6) in ordinary space, with the u_n as products of Hermite functions, have the unique property that their form is preserved in the special class of expansions governed by (2.7). Such form invariance can be considered as an unusual condition on ψ, more restrictive than what is commonly imposed on free particles; this makes the spectrum discrete, thus resolving the paradox. Nevertheless the 'Hermite packets' (4.6) form a complete set in terms of which any ψ can be expanded. The Hermite functions may be compared to the Airy functions, which generate wavepackets with the special property that $|\psi|^2$ for a free particle preserves its form in a uniformly accelerated reference frame (Berry and Balazs 1979, Greenberger 1980).

Other cases in which the motion is conservative in both reference frames occur when the potential $V(\boldsymbol{r})$ has the form γ/r^2 (inverse cube force), $\boldsymbol{C}\cdot\boldsymbol{r}/r^3$ (dipole field) and $\boldsymbol{r}\cdot\mathbf{T}\cdot\boldsymbol{r}/r^4$ where γ is a constant scalar, $\boldsymbol{C}$ a constant vector, and $\mathbf{T}$ a constant tensor; the last term of (3.1) is then obviously time-independent because $l(t)$ cancels.

5.2. One-dimensional expanding box, or continuously stretched quantum string

This system is the simplest example of a particle in a hard-walled expanding cavity, and can easily be generalised to an N-dimensional parallelepiped. The potential is

$$\begin{aligned} V(\rho)&=0, \qquad 0<\rho<1 \\ V(\rho)&=\infty, \qquad \rho\leqslant 0,\ \rho\geqslant 1. \end{aligned} \tag{5.1}$$

We shall not discuss the classical motion in detail, but draw attention to the fact that, for sufficiently small values of the constant $\mathscr{H}$, repeated reflection can occur not only at the walls $\rho=0$ and $\rho=1$ but also at intermediate ρ values (those for which $\mathscr{H}=\frac{1}{2}k\rho^2$).

The quantum mechanical expanding modes (solutions of 4.5) can be expressed in terms of parabolic cylinder functions (see e.g. Gradshteyn and Ryzhik 1965):

$$u_\nu(\rho)=\text{constant}\{D_\nu(z)-D_\nu(-z)\}, \tag{5.2}$$

where

$$z\equiv(4mk/\hbar^2)^{1/4}\rho, \tag{5.3}$$

and the order ν is related to the 'energy' $\mathscr{E}_\nu$ by

$$\mathscr{E}_\nu=(\nu+\tfrac{1}{2})\hbar(k/m)^{1/2}. \tag{5.4}$$

The solution (5.2) satisfies the boundary condition at $\rho=0$. At $\rho=1$ we require $u_\nu(1)=0$, and this imposes a discrete spectrum on ν and hence on $\mathscr{E}_\nu$. In the case $k=0$, of uniform linear expansion, or of no expansion at all, u_n is a simple trigonometric function and $\mathscr{E}_n=n^2\pi^2\hbar^2/2m$.

5.3. Expanding spherical cavity

This is the case studied by Klein and Mulholland (1978). They found, almost by accident, that for the repeated reflections of a particle from the sphere, a certain 'rebound function' is conserved, provided the expansion takes place in accordance with (2.7). It is now clear and not difficult to prove that, for classical motion, this conservation can be considered as a consequence of the conservation of the Hamiltonian $\mathscr{H}$ of (3.2), cf appendix.

Quantum mechanically, the expanding modes for this separable system can be labelled by three indices j, n, s and in spherical polar coordinates they may be written

$$u_{jns}(\rho) = (F_{jn}(\zeta)/\sqrt{\zeta})\, e^{is\phi}\, P_j^s(\cos\theta), \tag{5.5}$$

where

$$\zeta \equiv \rho(2m\mathscr{E}_{jn}/\hbar^2)^{1/2}. \tag{5.6}$$

The equation for the radial functions F_{jn} is found to be

$$\frac{d^2F_{jn}}{d\zeta^2} + \frac{1}{\zeta}\frac{d}{d\zeta} + \{1 - \kappa_{jn}\zeta^2 + (j+\tfrac{1}{2})^2/\zeta^2\}F_{jn} = 0, \tag{5.7}$$

where

$$\kappa_{jn} \equiv k\hbar^2/4m\mathscr{E}_{jn}. \tag{5.8}$$

The boundary conditions for a sphere of unit scaled radius ρ demand that

$$F_{jn}(0) = F_{jn}((2m\mathscr{E}_{jn}/\hbar^2)^{1/2}) = 0 \tag{5.9}$$

and determine the eigenvalues $\mathscr{E}_{jn}$.

For the special case $k = 0$, where the radial expansion is uniform, the solutions of (5.7) are elementary functions, since then F satisfies a Bessel equation with half-integer order, namely

$$F_{nj}(\zeta) = \text{constant}\ J_{j+1/2}(\zeta). \tag{5.10}$$

The eigenvalues are seen to be simply related to the zeros of these Bessel functions, as for a non-expanding sphere.

6. Expanding ensembles in statistical mechanics

Since the Hamiltonian $\mathscr{H}$ of (3.2) is time independent, we can imagine an ensemble of classical systems with a stationary distribution in $(\boldsymbol{\rho}, \boldsymbol{\pi})$ phase space, depending on $\mathscr{H}(\boldsymbol{\rho}, \pi; k)$. In the original $(\boldsymbol{r}, \boldsymbol{p})$ phase space the corresponding distribution is not stationary because there $\mathscr{H}$ is a function of time through the l-dependence of (3.4); it describes a non-equilibrium ensemble expanding with the force field. The analogous quantum mechanical ensemble, which we shall not consider further, would have a density matrix describing a mixture of states, each of which is one of the expanding modes (4.6).

Each such 'expanding ensemble' is specified by a function $G(\mathscr{H})$, in terms of which its distribution function in $(\boldsymbol{r}, \boldsymbol{p})$ is given by

$$f(\boldsymbol{r}, \boldsymbol{p}, t) = \{G[l^2H(\boldsymbol{r}, \boldsymbol{p}, l) - ll'\boldsymbol{r}\cdot\boldsymbol{p} + \tfrac{1}{2}mar^2]\}\Big/\left(\iint d^N\boldsymbol{r}\, d^N\boldsymbol{p}\, G[l^2H - ll'\boldsymbol{r}\cdot\boldsymbol{p} + \tfrac{1}{2}mar^2]\right). \tag{6.1}$$

In writing this formula we have used the fact that the transformation from $(\boldsymbol{\rho}, \boldsymbol{\pi})$ to $(\boldsymbol{r}, \boldsymbol{p})$ via (2.2) and (3.3) has Jacobian unity. It is unrealistic to imagine inter-particle interactions which scale with time in the special way envisaged in this paper, and so henceforth we restrict attention to the case where (6.1) describes ensembles of $\mathcal{N}$ non-interacting particles confined in an expanding (three-dimensional) vessel whose walls give rise to the potential $V(\boldsymbol{r}/l)$ in (1.1). Even with this restriction, the ensembles (6.1) do not describe homogeneous systems: in the canonical case, for example, for which $G=\exp(-\beta\mathcal{H})$, the spatial density varies radially as $\exp[-\frac{1}{2}\beta k r^2/l(t))^2]$ (as can be verified by integrating $f(\boldsymbol{r}, \boldsymbol{p}, t)$ over $\boldsymbol{p}$ and using (2.10*c*)), and the velocity distribution is only locally Maxwellian, with a mean radial velocity varying as $(l'/l)\boldsymbol{r}$.

We investigate the possibility of establishing thermodynamic analogies for the non-stationary ensemble averages obtained by integrating functions of $(\boldsymbol{r}, \boldsymbol{p})$ weighted by the distribution function $f(\boldsymbol{r}, \boldsymbol{p}, t)$. These averages will be evaluated by relating them to time-independent ensemble averages for phase functions of $\boldsymbol{\rho}$ and $\boldsymbol{\pi}$. Ensemble averages will be denoted by overbars.

Consider first the *internal energy* per particle, denoted by $U/\mathcal{N}$, corresponding to the average value of H. From (3.5), together with $\overline{\boldsymbol{\rho}\cdot\boldsymbol{\pi}}=0$ which follows from symmetry, we obtain

$$U/\mathcal{N} \rightleftharpoons (\overline{\mathcal{H}}-k\overline{\rho^2})/l^2+\tfrac{1}{2}ma\overline{\rho^2}, \tag{6.2}$$

where we use the symbol $\rightleftharpoons$ to denote the relation between a thermodynamic quantity and its statistical mechanical analogue (cf Tolman 1938). This has the same form as the quantal expectation value (4.8) and may be regarded as its classical analogue. Clearly, the internal energy decreases as the vessel expands.

Similarly, the correspondence for *pressure* P should be

$$P \rightleftharpoons -\overline{\partial H/\partial\Omega}. \tag{6.3}$$

where the *volume* Ω in the vessel varies with l and a geometrical constant K,

$$\Omega = Kl^3, \tag{6.4}$$

while H depends parametrically on l by (1.1). Thus

$$P \rightleftharpoons -\frac{\mathcal{N}}{3l^2K}\overline{\frac{\partial H}{\partial l}}=\frac{\mathcal{N}}{3l^2\Omega}(2\overline{V(\boldsymbol{\rho})}+\overline{\boldsymbol{\rho}\cdot\partial V(\boldsymbol{\rho})/\partial\boldsymbol{\rho}}). \tag{6.5}$$

Substituting for V with the aid of (3.2), we obtain

$$P \rightleftharpoons \frac{\mathcal{N}}{3l^2\Omega}\left(2(\overline{\mathcal{H}}-k\overline{\rho^2})-\overline{\pi^2}/m+\overline{\boldsymbol{\rho}\cdot\frac{\partial}{\partial\boldsymbol{\rho}}\mathcal{H}}\right). \tag{6.6}$$

The last two terms cancel by virtue of the generalised equipartition theorem of Tolman (1938) for the ensemble in $\boldsymbol{\rho}$, $\boldsymbol{\pi}$ space, which applies because $\pi^2/m=\boldsymbol{\pi}\cdot\partial\mathcal{H}/\partial\boldsymbol{\pi}$ and the components of $\boldsymbol{\rho}$ are confining coordinates (this theorem holds for any ensemble of the type 6.1). Substitution for $\mathcal{H}$ from (3.2) and using the stipulation that $V=0$ inside the vessel give, finally,

$$P \rightleftharpoons (\mathcal{N}/3l^2\Omega)(\overline{\pi^2}/m-k\overline{\rho^2}). \tag{6.7}$$

Next we consider the *temperature* T, for which the generalised equipartition theorem suggests the correspondence

$$k_{\mathrm{B}}T \rightleftharpoons \tfrac{1}{3}\overline{\boldsymbol{p}\cdot\partial H/\partial\boldsymbol{p}}, \tag{6.8}$$

where k_B denotes Boltzmann's constant. With (3.3), (2.2) and (2.10*c*) this becomes

$$k_B T \rightleftharpoons (1/3l^2)[\overline{\pi^2}/m + (mal^2 - k)\overline{\rho^2}]. \tag{6.9}$$

This temperature is a property of the system as a whole and is different from the uniform local temperature inferred from the local velocity distribution (Maxwellian in the case of a canonical ensemble) as seen in a frame moving with local expansion.

The quantities *U*, *P*, *T*, which have just been calculated, can be considered as analogous to the corresponding quantities in ordinary equilibrium thermodynamics only if there exists an analogy for the second law of thermodynamics. This requires that if d refers to differences between quantities belonging to ensembles whose parameters (e.g. *k*) differ infinitesimally, then the quantity

$$(1/T)(\mathrm{d}U + P\,\mathrm{d}\Omega) \tag{6.10}$$

must be the differential of a function *S* which of course is the entropy of the system. From (6.2), (6.7) and (6.9), and using (6.4), we obtain

$$\frac{1}{T}(\mathrm{d}U + P\,\mathrm{d}\Omega) \rightleftharpoons \frac{3}{2}\frac{k_B}{\{\frac{1}{2}\overline{\pi^2}/m + \frac{1}{2}\overline{\rho^2}(mal^2 - k)\}}[\mathrm{d}\{\tfrac{1}{2}\overline{\pi^2}/m - \tfrac{1}{2}k\overline{\rho^2}\} + l^2\,\mathrm{d}\{\tfrac{1}{2}ma\overline{\rho^2}\}]. \tag{6.11}$$

Since this is not, in general, a perfect differential, our tentative thermodynamic analogues are thus seen to be generally unsound. They are vindicated, however, for the very special expansion when $a = 0$, which corresponds to the vessel's surface area increasing at a constant rate (cf 2.7) and for which (cf 2.8)

$$b^2 = -k/m, \qquad a = 0, \qquad l(t) = (2bt + c)^{1/2}. \tag{6.12}$$

For this case, (6.11) does define a function of state, namely

$$S \rightleftharpoons \mathcal{N} k_B \ln\{\tfrac{1}{2}\overline{\pi^2}/\mathrm{m} + \tfrac{1}{2}mb^2\overline{\rho^2}\}^{3/2} + \text{constant}. \tag{6.13}$$

Moreover, this entropy, depending only on averages in the stationary ensemble, remains constant during the expansion, and the original system may be said to undergo a *finite rate isentropic process.* In addition, (6.7) and (6.9) show that when $a = 0$ the system obeys the ideal gas equation of state at every instant, that is

$$P\Omega = \mathcal{N} k_B T, \tag{6.14}$$

and the entropy can be written as

$$S = \mathcal{N} k_B \ln(\Omega T^{3/2}), \tag{6.15}$$

which has the same form as for an ideal gas in equilibrium thermodynamics. Further it follows from (6.9) that the temperature of the system is inversely proportional to the surface area of the vessel.

For these conclusions to represent more than mathematical analogies, the ensembles (6.1) (with $a = 0$) must be physically realisable. One way to achieve this for the canonical case with $G = \exp(-\beta\mathcal{H})$ might be to prepare the gas in an ordinary canonical distribution by contact with a heat reservoir, with the vessel not expanding, then insulate the vessel and then expand it in accordance with (2.7) with $a = 0$. The sudden onset of the expansion would initiate irreversible processes such as damped sound waves, and there is the possibility that these transient effects could provide the mechanism to alter the distribution to (6.1). We are not able to prove that this would happen.

A consequence of the constancy of entropy, easily obtained from (6.8) and (6.9) with $a = 0$, is

$$l^2\overline{p^2} = \text{constant}. \tag{6.16}$$

A result corresponding to this, but as a *time average* for the free flight of a particle between wall rebounds, with the same constant for successive free paths, has been obtained previously (Klein and Mulholland 1978, equation (5.12)). Also, constancy of the total entropy is consistent with the uniformity of local kinetic temperature mentioned above, since in the absence of other dissipative effects, uniformity of temperature implies no heat conduction, no entropy flux, and no local entropy production.

7. Concluding remarks

We have considered systems changing in time in consequence of a *finite* rate of change of an external parameter, namely the linear scale factor $l(t)$. For changes in accordance with (2.7), a dilating frame of reference, and a recalibration of clocks, can be found, in which classical trajectories are determined by the stationary Hamiltonian $\mathscr{H}$ (equation 3.2), and the quantum system possesses well defined time-independent wavefunctions u_n and eigenvalues $\mathscr{E}_n$ satisfying (4.5). $\mathscr{H}$, u_n and $\mathscr{E}_n$ do depend on the expansion rate, as given by (2.7), but only through its constant coefficients as embodied in k (equation 2.8). $\mathscr{H}$ is an adiabatic invariant, not only in respect of slow changes of l, for which the concept has been formulated (cf Whittaker 1953), but also in respect of changes at finite rate, provided these are in accordance with (2.7). The constant of motion is given explicitly in terms of the original phase-space variables by (3.4).

Although governed by a stationary Hamiltonian, motion in the expanding force field is different from that in the non-expanding field, because of the extra potential $\frac{1}{2}k\rho^2$ in (3.2). The differences can be fundamental, in that expansion can alter the topology of the orbits. For example, if the original potential V describes two uncoupled harmonic oscillators with frequencies ω_1 and ω_2, where ω_1/ω_2 is rational, the orbit for an unexpanding system (l = constant) is a closed plane curve; for the expanding system, the addition of $\frac{1}{2}k\rho^2$ changes the frequency ratio to $(\omega_1^2+k/m)^{1/2}/(\omega_2^2+k/m)^{1/2}$, which will almost always be irrational so that the orbit never closes (and indeed fills a rectangle in $\boldsymbol{\rho}$ space). A more profound difference would arise if integrable motion could be rendered chaotic (Berry 1978) by the addition of $\frac{1}{2}k\rho^2$, with consequent change in the form of the eigenfunctions from regular to irregular (Berry 1977). (This cannot happen if V separates in Cartesian coordinates or in polar coordinates whose origin is the centre of expansion.)

It should be possible to generalise results to relativistic motion, in particular to the wave optics of expanding cavities, and to the case of anisotropic expansion.

Appendix

A particle moving classically in an expanding spherical vessel of radius $l = l(t)$ is free except for elastic reflections from the hard wall at $\rho = 1$. The spherical symmetry implies that angular momentum about the centre is conserved; let its magnitude, per unit mass, be $h \equiv |\boldsymbol{r} \wedge \boldsymbol{v}|$, where $\boldsymbol{v}$ is the velocity of the particle. If now the expansion follows (2.7), the Hamiltonian $\mathscr{H}$ of (2.2) is also conserved; close to the wall at $\rho = 1$

(that is, just before and after a reflection),

$$\mathscr{H} = \tfrac{1}{2}\pi^2/m + \tfrac{1}{2}k.$$

With (3.3) and (2.2) the right-hand side equals

$$\tfrac{1}{2}mh^2 + \tfrac{1}{2}mr^2(\hat{\boldsymbol{r}}\cdot\boldsymbol{v} - l')^2 + \tfrac{1}{2}k,$$

where $\hat{\boldsymbol{r}} \equiv \boldsymbol{r}/r = \boldsymbol{\rho}$ on impact, and since this expression is constant it follows also that for successive reflections

$$(\hat{\boldsymbol{r}}\cdot\boldsymbol{v} - l')^2/|\hat{\boldsymbol{r}}\wedge\boldsymbol{v}|^2$$

is conserved. This quantity is the square of the 'rebound function' introduced by Klein and Mulholland (1978), and it is remarkable that it contains speeds and angles only. The result means that

$$(v_2\cos\chi_2 + l')/v_2\sin\chi_2 = (v_1\cos\chi_1 - l')/v_1\sin\chi_1 = \text{constant},$$

where v and χ are the speed and angle at any rebound, the subscripts 1 and 2 refer to incidence and reflection, and l' is the instantaneous rate of radial expansion of the sphere. While the equality of the two ratios for a given rebound is an elementary result (also valid relativistically), what is interesting here is that all pairs of ratios have the same single value for all successive reflections.

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