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The spreading of wavepackets in quantum mechanics

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Abstract. For a wavepacket representing a particle subject to a conservative force, consideration is given to the evolution in time of the mean position and momentum and to the evolution of the spread of these quantities as measured by the mean square deviation from the mean. A closed system of equations involving these spreads is obtained by expanding the potential in powers about the mean position and by neglecting terms of third order or higher in the deviations from the mean, an approximation appropriate when the force does not vary too much over the width of the packet. These equations are solved in terms of the trajectories of a classical time-dependent oscillator. These trajectories can be found by differentiation of the trajectories for the force under consideration.

In more than one dimension, or for more than one particle, the appropriate generalisation of the spread is the set of second-order correlations, e.g. $\langle (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle)\rangle$. Again the equations for their evolution when higher correlations are neglected are solved in terms of classical trajectories. The equations for the evolution of these quantum correlations are identical to those for corresponding averages over clusters of classical particles, but quantum effects do appear in matching to the initial conditions. Some generalisations are briefly considered.

1. Introduction

Quantum wavepackets follow classical trajectories provided the force acting does not change significantly across the width of the packet. This follows from Ehrenfest's theorem (e.g. Messiah 1961, ch VI, § 2), which states that for a particle of mass m under a force $\boldsymbol{F}(\boldsymbol{x})$ derived from a potential $V(\boldsymbol{x})$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \boldsymbol{x} \rangle = \frac{1}{m}\langle \boldsymbol{p} \rangle, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle \boldsymbol{p} \rangle = \langle \boldsymbol{F} \rangle. \tag{1.1}$$

If $\langle \boldsymbol{F}(\boldsymbol{x})\rangle \approx \boldsymbol{F}(\langle \boldsymbol{x} \rangle)$, then $\langle \boldsymbol{x} \rangle$ will follow the classical trajectory. Thus the smaller the spread in position of the packet, the more closely will it follow the classical path. Unless the spread in momentum is also small, however, the packet will quickly spread in spatial extent.

In order to calculate how well a wavepacket will follow the classical trajectory, it is necessary to calculate the way the spread of the packet changes as the packet moves. In one dimension, the spread is conveniently measured by the root-mean-square deviation from the mean position, $\Delta x = \langle (x - \langle x \rangle)^2 \rangle^{1/2}$. Indeed it is precisely this which is required to calculate a first correction to the trajectory.

Messiah (1961, ch VI, § 3) treats this topic in the one-dimensional case by expanding the potential in powers of $x - \langle x \rangle$, and this is the procedure that will be adopted here.

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Unfortunately, although presented as being valid for an arbitrary but slowly varying potential, his results are not generally valid (see Appendix). They are valid for quadratic potentials, for which there is a considerable recent literature (e.g. Askar and Weiner 1971, Hasse 1978, Remaud and Hernandez 1980).

We will require rates of change of quantities of the form $\langle(a-\langle a\rangle)(b-\langle b\rangle)\rangle$, where a and b are Hermitian operators. This expectation value can also be written as $\langle ab\rangle - \langle a\rangle\langle b\rangle$, and hence

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}&\langle(a-\langle a\rangle)(b-\langle b\rangle)\rangle\\ &= \mathrm{i}\hbar^{-1}\langle[H,a]b+a[H,b]-[H,a]\langle b\rangle-\langle a\rangle[H,b]\rangle\\ &= \mathrm{i}\hbar^{-1}\langle(a-\langle a\rangle)[H,b]-[H,a](b-\langle b\rangle)\rangle. \qquad (1.2)\end{aligned}$$

Since $\langle a-\langle a\rangle\rangle=0$, $[H,b]$ may be replaced by $[H,b]-\langle[H,b]\rangle$ and similarly for $[H,a]$. These calculations would be a little simpler in the Heisenberg picture but there is, of course, no essential difference.

2. Wavepacket for a single particle in one dimension

Let x and p represent the position and momentum observables and write $X=x-\langle x\rangle$, $P=p-\langle p\rangle$. The Hamiltonian is $H=(2m)^{-1}p^2+V(x)$. Using $[H,x]=-\mathrm{i}\hbar p/m$ and $[H,p]=\mathrm{i}\hbar V'$, equation (1.2) gives

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\langle X^2\rangle = m^{-1}\langle Xp+pX\rangle = m^{-1}\langle XP+PX\rangle,\\ &\frac{\mathrm{d}}{\mathrm{d}t}\langle XP\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle PX\rangle = \langle m^{-1}P^2-XV'\rangle, \qquad (2.1)\\ &\frac{\mathrm{d}}{\mathrm{d}t}\langle P^2\rangle = -\langle PV'+V'P\rangle.\end{aligned}$$

A closed system of equations is obtained if one expands the force through

$$V'(x)=v'+v''X+\tfrac{1}{2}v'''X^2+\ldots \qquad (2.2)$$

where $v'=V'(\langle x\rangle)$, $v''=V''(\langle x\rangle)$ and $v'''=V'''(\langle x\rangle)$. Then $V'-\langle V'\rangle=v''X$ where we ignore, at this stage, terms involving third or higher derivatives of V, since on insertion in (2.1) they will give third-order correlations, e.g. $\langle X^3\rangle$ or $\langle PX^2\rangle$. Thus

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\langle P^2\rangle = -v''\langle PX+XP\rangle = -mv''\frac{\mathrm{d}}{\mathrm{d}t}\langle X^2\rangle,\\ &\frac{1}{2}m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle X^2\rangle = m^{-1}\langle P^2\rangle - v''\langle X^2\rangle.\end{aligned} \qquad (2.3)$$

Write $\chi=\langle X^2\rangle$, $\omega=m^{-2}\langle P^2\rangle$ and $\phi(t)=m^{-1}v''$. To a sufficient approximation, v'' is known as a function of t from the classical trajectory when $\langle x\rangle$ and $\langle p\rangle$ are given at $t=0$. Equation (2.3) becomes

$$\dot{\omega}=-\phi\dot{\chi}, \qquad \tfrac{1}{2}\ddot{\chi}=\omega-\phi\chi. \qquad (2.4)$$

This pair of coupled differential equations for χ, ω yields a third-order linear differential equation in χ alone:

$$\tfrac{1}{2}\dddot{\chi} + 2\phi\dot{\chi} + \dot{\phi}\chi = 0. \tag{2.5}$$

With the substitution (Kamke 1959) $\chi = uv$, this equation can be written as

$$(v\, \mathrm{d}/\mathrm{d}t + 3\dot{v})(\ddot{u} + \phi u) + (u\, \mathrm{d}/\mathrm{d}t + 3\dot{u})(\ddot{v} + \phi v) = 0.$$

Hence if u and v are any two solutions of $\ddot{u} + \phi u = 0$, then $\chi = uv$ will satisfy (2.5). If u and v are linearly independent, then u^2, uv, v^2 form a complete basis for solutions of (2.5).

Let u and v be chosen such that $u(0) = 1$, $\dot{u}(0) = 0$ and $v(0) = 0$, $\dot{v}(0) = 1$ and write $\chi = Au^2 + Buv + Cv^2$ where A, B, C are constants. Then $\dot{\chi} = 2Au\dot{u} + B(u\dot{v} + \dot{u}v) + 2Cv\dot{v}$ and, using $\omega = \frac{1}{2}\ddot{\chi} + \phi\chi$, $\omega = A\dot{u}^2 + B\dot{u}\dot{v} + C\dot{v}^2$. Then the boundary conditions on u, v at $t = 0$ give $A = \chi_0 := \langle X^2 \rangle_{t=0}$, $B = \dot{\chi}_0 := m^{-1}\langle XP + PX \rangle_{t=0}$, $C = \omega_0 := m^{-2}\langle P^2 \rangle_{t=0}$. The system of equations

$$\begin{aligned} \chi &= \chi_0 u^2 + \dot{\chi}_0 uv + \omega_0 v^2, \\ \dot{\chi} &= 2\chi_0 u\dot{u} + \dot{\chi}_0(u\dot{v} + \dot{u}v) + 2\omega_0 v\dot{v}, \\ \omega &= \chi_0 \dot{u}^2 + \dot{\chi}_0 \dot{u}\dot{v} + \omega_0 \dot{v}^2, \end{aligned} \tag{2.6}$$

constitute a solution to the problem of the time evolution of the spread in position and momentum of a wavepacket as it follows approximately a classical trajectory.

3. Obtaining the quantum spreading from the classical trajectory

Consider two classical particles of mass m at neighbouring points x_1 and x_2, each subject to the potential $V(x)$ but with no interaction between the two. Thus $m\ddot{x}_1 = -V'(x_1)$, $m\ddot{x}_2 = -V'(x_2)$. Expanding the potential as $V'(x_2) \approx V'(x_1) + (x_2 - x_1)V''(x_1)$ and writing $y := x_2 - x_1$ yields $\ddot{y} = -\phi(t)y$. It is now clear that the functions u and v required to calculate the evolution of a quantum packet can be obtained from the classical trajectory.

Let $x(a, b, t)$ be a classical trajectory such that $m\ddot{x} = -V'(x)$ and $x(a, b, 0) = a$, $\dot{x}(a, b, 0) = b$. Define $u(t) := \partial x/\partial a$, $v(t) := \partial x/\partial b$. Then $\ddot{u} + \phi u = 0$, $\ddot{v} + \phi v = 0$ and $u(0) = 1$, $\dot{u}(0) = 0$, $v(0) = 0$, $\dot{v}(0) = 1$. These are precisely the functions needed for insertion into (2.6) to calculate the evolution of a packet.

4. A correction to the classical trajectory

Having found χ, a correction can be made to the trajectory of $\langle x \rangle$ using

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x \rangle = -V'(\langle x \rangle) - \tfrac{1}{2}\chi V'''(\langle x \rangle). \tag{4.1}$$

This is the equation for classical motion under a given time-dependent potential, but here it is meaningful to include only terms linear in χ in the solution. Write $\langle x \rangle = \xi + \eta$, where $m\ddot{\xi} = -V'(\xi)$ and ξ satisfies the given initial conditions for $\langle x \rangle$. Then (4.1) becomes $\ddot{\eta} + \phi\eta = -\zeta(t)$, where $\zeta(t) = (2m)^{-1}\chi V'''(\xi)$ and terms quadratic in χ or η

have been dropped. The solution of this with $\eta(0)=\dot{\eta}(0)=0$ is

$$\eta=\int_0^t [u(t)v(t')-v(t)u(t')]\zeta(t')\,\mathrm{d}t'. \tag{4.2}$$

5. Inequalities and invariants

The quantities χ, $\dot{\chi}$, ω do not change independently. Equations (2.4) yield $(\mathrm{d}/\mathrm{d}t)(4\chi\omega-\dot{\chi}^2)=0$. Thus $h^2:=\chi\omega-\frac{1}{4}\dot{\chi}^2$ is constant. Application of the Schwarz inequality (Merzbacher 1970, ch 8, § 6, first equation on p 160) shows that

$$4\langle X^2\rangle\langle P^2\rangle\geqslant\langle XP+PX\rangle^2+|\langle XP-PX\rangle|^2=\hbar^2+\langle XP+PX\rangle^2.$$

Hence

$$4\chi\omega-\dot{\chi}^2\geqslant(\hbar/m)^2. \tag{5.1}$$

This shows that, although $\chi=(\alpha u+\beta v)^2$ is a solution of (2.5), it could not fit the boundary conditions, since this would require $4\chi_0\omega_0=\dot{\chi}_0^2$.

Writing $\rho=\chi^{1/2}$, so that ρ is the root-mean-square deviation from the mean position, the definition of h gives

$$\rho^3(\ddot{\rho}+\phi\rho)=h^2. \tag{5.2}$$

The close connection between this equation and the equation $\ddot{q}+\phi(t)q=0$ for the motion of a 'time-dependent harmonic oscillator' has been studied for some time and particularly recently in connection with dynamical invariants (Reid and Ray 1980, Korsch 1979, and references contained in these). Equations (2.6) can be inverted, using $u\dot{v}-\dot{u}v=1$, to give

$$\begin{gathered}\chi_0=\chi\dot{v}^2-\dot{\chi}v\dot{v}+\omega v^2, \qquad \dot{\chi}_0=-2\chi\dot{u}\dot{v}+\dot{\chi}(u\dot{v}+\dot{u}v)-2\omega uv,\\ \omega_0=\chi\dot{u}^2-\dot{\chi}u\dot{u}+\omega u^2.\end{gathered} \tag{5.3}$$

The right-hand sides of these equations are dynamical invariants for any solutions u and v of $\ddot{q}+\phi q=0$.

The evolution in time of the spread of a one-dimensional quantum wavepacket (to the approximation considered here) thus provides a realisation of a time-dependent oscillator; but whereas in the literature $\ddot{q}+\phi q=0$ has been thought of as the equation of motion and (5.2) as an auxiliary equation useful in its analysis, here the roles of the two equations are reversed. We will see that the spread of a cluster of classical particles satisfies the same equations.

6. Wavepacket for a single particle in more than one dimension

Denote the position coordinates by x_i and the momenta by p_i, and put $X_i=x_i-\langle x_i\rangle$, $P_i=p_i-\langle p_i\rangle$. Instead of the single quantity $\langle X^2\rangle$ to represent the spread of the packet, we now consider the tensor $\langle X_iX_j\rangle$. Assuming $H=(2m)^{-1}\Sigma_i p_i^2+V(\boldsymbol{x})$, where $\boldsymbol{x}$ signifies the set $x_1, x_2, \ldots$, it follows that $[H, x_j]=(\hbar/\mathrm{i}m)p_j$ and $[H, p_j]=\mathrm{i}\hbar V_j$ where

$V_j := \partial V/\partial x_j$. Equation (1.2) then gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X_iX_j\rangle = m^{-1}\langle X_iP_j + P_iX_j\rangle, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle X_iP_j\rangle = m^{-1}\langle P_iP_j\rangle - \langle X_iV_j\rangle,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P_iX_j\rangle = m^{-1}\langle P_iP_j\rangle - \langle V_iX_j\rangle, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle P_iP_j\rangle = -\langle P_iV_j + V_iP_j\rangle. \tag{6.1}$$

Approximation of $V_i(\boldsymbol{x})$ by $v_i + X_jv_{ij}$ (repeated indices to be summed) then leads to the closed system

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X_iX_j\rangle = m^{-1}\langle X_iP_j + P_iX_j\rangle, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle X_iP_j\rangle = m^{-1}\langle P_iP_j\rangle - \langle X_iX_k\rangle v_{kj},$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P_iX_j\rangle = m^{-1}\langle P_iP_j\rangle - \langle X_kX_j\rangle v_{ik}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle P_iP_j\rangle = -(\langle P_iX_k\rangle v_{kj} + \langle X_kP_j\rangle v_{ik}). \tag{6.2}$$

The required solutions of this system can be constructed from the solutions of the simpler set

$$\ddot{u}_i + \phi_{ij}u_j = 0 \tag{6.3}$$

where $\phi_{ij} := m^{-1}v_{ij}$. If u_i and v_i are any two sets of solutions of (6.3) then $\langle X_iX_j\rangle = u_iv_j$, $\langle X_iP_j\rangle = u_i\dot{v}_j + C\delta_{ij}$, $\langle P_iX_j\rangle = \dot{u}_iv_j - C\delta_{ij}$, $\langle P_iP_j\rangle = \dot{u}_i\dot{v}_j$ satisfy (6.2). In order to satisfy the boundary conditions at $t=0$, let u_i^k, v_i^k be a basis set of solutions of (6.3) such that $u_i^k(0) = \delta_i^k$, $\dot{u}_i^k(0) = 0$ and $v_i^k(0) = 0$, $\dot{v}_i^k(0) = \delta_i^k$. Then

$$\begin{aligned}
\langle X_iX_j\rangle &= A_{kl}u_i^ku_j^l + B_{kl}(u_i^kv_j^l + u_j^kv_i^l) + C_{kl}v_i^kv_j^l,\\
m^{-1}\langle X_iP_j\rangle &= A_{kl}u_i^k\dot{u}_j^l + B_{kl}(u_i^k\dot{v}_j^l + \dot{u}_j^kv_i^l) + \tfrac{1}{2}\mathrm{i}\hbar m^{-1}\delta_{ij} + C_{kl}v_i^k\dot{v}_j^l,\\
m^{-1}\langle P_iX_j\rangle &= A_{kl}\dot{u}_i^ku_j^l + B_{kl}(\dot{u}_i^kv_j^l + u_j^k\dot{v}_i^l) - \tfrac{1}{2}\mathrm{i}\hbar m^{-1}\delta_{ij} + C_{kl}\dot{v}_i^kv_j^l,\\
m^{-2}\langle P_iP_j\rangle &= A_{kl}\dot{u}_i^k\dot{u}_j^l + B_{kl}(\dot{u}_i^k\dot{v}_j^l + \dot{u}_j^k\dot{v}_i^l) + C_{kl}\dot{v}_i^k\dot{v}_j^l,
\end{aligned} \tag{6.4}$$

satisfy (6.2), and putting $t=0$ gives

$$A_{ij} = \langle X_iX_j\rangle_0, \qquad 2mB_{ij} = \langle X_iP_j + P_iX_j\rangle_0 + e_{ijk}\langle L_k\rangle_0,$$
$$m^2C_{ij} = \langle P_iP_j\rangle_0, \tag{6.5}$$

where $\boldsymbol{L} = \boldsymbol{X}\times\boldsymbol{p}$ and we have used $\langle X_iP_j - P_iX_j\rangle = \mathrm{i}\hbar\delta_{ij} + e_{ijk}\langle L_k\rangle$. Thus A and C are symmetric matrices, but B is symmetric if and only if the packet has no angular momentum about its centroid at $t=0$.

The functions u_i^k, v_i^k can be obtained from the classical trajectory. Let $\boldsymbol{x}(\boldsymbol{a},\boldsymbol{b},t)$ satisfy Newton's equation of motion $m\ddot{x}_i = -\partial V/\partial x_i$ and the initial conditions $\boldsymbol{x}(\boldsymbol{a},\boldsymbol{b},0) = \boldsymbol{a}$ and $\dot{\boldsymbol{x}}(\boldsymbol{a},\boldsymbol{b},0) = \boldsymbol{b}$. Define $u_i^k = \partial x_i/\partial a_k$ and differentiate Newton's equation with respect to a_k. Hence $m\ddot{u}_i^k = -u_j^k\,\partial^2V/\partial x_i\,\partial x_j$ with initial conditions at $t=0$, $u_i^k(0) = \delta_i^k$ and $\dot{u}_i^k(0) = 0$. Similarly defining $v_i^k = \partial x_i/\partial b_k$ leads to $m\ddot{v}_i^k = -v_j^k\,\partial^2V/\partial x_i\,\partial x_j$ with $v_i^k(0) = 0$, $\dot{v}_i^k(0) = \delta_i^k$.

7. Spreading of clusters of classical particles

Consider a cluster of n-identical classical particles each of mass m and subject to the same potential $V(\boldsymbol{x})$ so that the μth particle, at position x_i^μ, moves according to

$m\ddot{x}_i^\mu = -V_i(\boldsymbol{x}^\mu)$ where $V_i(\boldsymbol{x}) = \partial V(\boldsymbol{x})/\partial x_i$. Define mean values by summing over the particles in the cluster; thus $\langle x_i \rangle := n^{-1}\Sigma_\mu x_i^\mu$. Then $\mathrm{d}\langle x_i\rangle/\mathrm{d}t = n^{-1}\Sigma_\mu \dot{x}_i^\mu =: \langle \dot{x}_i\rangle$ and $\mathrm{d}^2\langle x_i\rangle/\mathrm{d}t^2 = n^{-1}\Sigma_\mu \ddot{x}_i^\mu =: \langle \ddot{x}_i\rangle = -(mn)^{-1}\Sigma_\mu V_i(\boldsymbol{x}^\mu) =: m^{-1}\langle V_i\rangle$. Write $X_i := x_i - \langle x_i\rangle$ and expand $V_i(\boldsymbol{x})$ in powers about $\langle \boldsymbol{x}\rangle$: thus $V_i(\boldsymbol{x}) = v_i + v_{ij}X_j + \frac{1}{2}v_{ijk}X_jX_k + \ldots$, where $v_i = V_i(\langle \boldsymbol{x}\rangle)$, $v_{ij} = V_{ij}(\langle \boldsymbol{x}\rangle)$, etc.

If we ignore correlations of third or higher orders we obtain the following equations for the second-order correlations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X_iX_j\rangle = \langle X_i\dot{X}_j + \dot{X}_iX_j\rangle,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X_i\dot{X}_j\rangle = \langle \dot{X}_i\dot{X}_j\rangle - m^{-1}\langle X_iV_j\rangle \approx \langle \dot{X}_i\dot{X}_j\rangle - m^{-1}\langle X_iX_k\rangle v_{kj}, \tag{7.1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \dot{X}_i\dot{X}_j\rangle = -m^{-1}\langle \dot{X}_iV_j + V_i\dot{X}_j\rangle \approx -m^{-1}(\langle \dot{X}_iX_k\rangle v_{kj} + \langle X_k\dot{X}_j\rangle v_{ik}).$$

These are identical in form to (6.2), and the solutions we obtained to those equations will serve here, the only difference being that the term in $\hbar$ in (6.4) is not needed to fit the boundary conditions here. In one dimension, only the symmetrised mixed correlation $\langle XP + PX\rangle$ is required to give a closed system of equations for the quantum case, and then there is no difference between the classical and quantum cases; no terms involving $\hbar$ appear. In more than one dimension $\langle X_iP_j\rangle$ and $\langle P_iX_j\rangle$ are required separately, and a term in $\hbar$ is unavoidable. This difference may be due to the absence of angular motion in one dimension.

8. Differential inequalities

From (5.1) follows the weaker inequality $\dot{\chi}^2 \leqslant 4\chi\omega$. In terms of $\Delta x := \chi^{1/2}$, that is, the root-mean-square deviation from the mean position, this gives $|\mathrm{d}(\Delta x)/\mathrm{d}t| \leqslant m^{-1}\Delta p$. It will now be shown that this is a special case of a more general inequality for the rate of change of the spread of any observable a.

Define $(\Delta a)^2 = \langle (a - \langle a\rangle)^2\rangle = \langle a^2\rangle - \langle a\rangle^2$. Equation (1.2) then gives

$$\frac{\mathrm{d}}{\mathrm{d}t}(\Delta a)^2 = \mathrm{i}\hbar^{-1}\langle (a - \langle a\rangle)[H, a] - [H, a](a - \langle a\rangle)\rangle.$$

The Schwarz inequality shows that $|\langle [(a - \langle a\rangle), \mathrm{i}[H, a]]\rangle| \leqslant 2\Delta a\ \Delta(\mathrm{i}[H, a])$ and hence

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\Delta a\right| \leqslant \Delta(\mathrm{i}\hbar^{-1}[H, a]). \tag{8.1}$$

This exact inequality is striking in its simplicity and in its close parallel to the Ehrenfest relation

$$\mathrm{d}\langle a\rangle/\mathrm{d}t = \mathrm{i}\hbar^{-1}\langle [H, a]\rangle.$$

I cannot see, however, how (8.1) can be usefully applied to the present problem. In the case of a single particle under the potential V, we have

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\Delta x_i\right| \leqslant m^{-1}\,\Delta p_i, \qquad \left|\frac{\mathrm{d}}{\mathrm{d}t}\Delta p_i\right| \leqslant \Delta V_i.$$

As well as the difficulty of dealing with coupled sets of inequalities, there is the weakness that the inequality (8.1) applies only to the *magnitude* of the rate of change and therefore cannot distinguish between a positive rate, which will allow a continuing increase in the spread, and a negative rate, for which the spread may oscillate.

9. Generalisations

Several generalisations of the work above suggest themselves but will not be fully worked out here. Third- and higher-order correlations may be considered. A closed set of equations can be obtained for the nth-order correlations if higher orders are neglected. If third-order correlations are to be taken into account, the equations for the second-order correlations are more complex than those considered above, and the solutions for the third-order correlations are required as input to these second-order equations. These high correlations can be used to improve the trajectory (i.e. the evolution of the first-order quantities).

Another generalisation is to consider the evolution of packets representing several interacting particles. Consider the case of two particles in one dimension with Hamiltonian $(2m_1)^{-1}p_1^2+(2m_2)^{-1}p_2^2+V(x_1,x_2)$. We have $\mathrm{d}\langle x_i\rangle/\mathrm{d}t=m_i^{-1}\langle p_i\rangle$ (no summation) and $\mathrm{d}\langle p_i\rangle/\mathrm{d}t=-\langle V_i\rangle$. Write $X_i:=x_i-\langle x_i\rangle$ and expand $V(x_1,x_2)=v+v_iX_i+\frac{1}{2}v_{ij}X_iX_j+\ldots$ where $v=V(\langle x_1\rangle,\langle x_2\rangle)$, etc. To a first approximation, $\langle x_i\rangle$ are determined as functions of t by the solution of the classical two-body problem with potential V. The development is formally similar to that of § 6 except that now the mass depends on the index i. This makes little difference, although the quantity $\phi_{ij}:=(m_i)^{-1}v_{ij}$ is now not symmetric in its indices.

Finally, one could consider non-conservative systems such as a particle in an electromagnetic field.

Appendix. On Messiah's discussion of the spreading of wavepackets

Messiah's equation VI.12 is correct, but he assumes that ε is constant. In fact $\mathrm{d}\varepsilon/\mathrm{d}t\approx(2m)^{-1}\langle p\rangle\chi V_{\mathrm{cl}}'''$. After a time t, ε will change by an amount of the order of $(2m)^{-1}\langle p\rangle\chi V_{\mathrm{cl}}'''t$. Writing $X=\langle p\rangle t/m$ for the mean distance travelled in that time, then unless $V_{\mathrm{cl}}'''X\ll V_{\mathrm{cl}}''$, the change in ε will be of the same order as the other term in VI.12, namely $V_{\mathrm{cl}}''\chi$. Unless V is essentially quadratic, the variation in ε must be taken into account, and this leads to the third-order equation (2.5) above.

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