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Classical distribution functions derived from Wigner distribution functions

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Abstract. A mapping which relates the Wigner phase-space distribution function associated with a given stationary quantum-mechanical wavefunction to a specific solution of the time-independent Liouville transport equation is obtained. Two examples are studied.

1. Introduction

There has been much concern about the classical limit of quantum mechanics. This limit may be accomplished in two steps: first one makes a mapping of the Wigner phase-space distribution function (WDF) to a classical phase-space distribution function (CDF) which still might depend on $\hbar$, and in a second step the $\hbar = 0$ limit is taken. Here we shall be interested in the first step, namely in a prescription which relates the WDF of a given stationary quantum mechanical wavefunction, a solution of the Schrödinger equation, to a specific solution of the Liouville equation, both subject to the same potential. We first present a short derivation of the expression for the CDF, discuss a few of its properties and then give two examples, one corresponding to a bound state and the second to a scattering state.

Our prescription for the CDF corresponds to taking averages of the WDF over classical trajectories. In the special case of linear or quadratic potentials the WDF coincides with the CDF [1, 2], as in this case the WDF already satisfies the Liouville equation. In the case in which the Wigner function is generated by a scattering solution of the Schrödinger equation, the CDF gives the classical limit, it describes individual trajectories corresponding to classical scattering.

Here we only consider problems in one degree of freedom. An extension which might be considered is semiclassical elastic and inelastic scattering of a particle by a two-body bound state. Using the mapping introduced here, essentially one expects to obtain the approximation introduced by Lee and Scully [3], except that, instead of describing the initial and final two-body bound states by a WDF [4], the corresponding CDF obtained through our prescription would have to be used.

2. The classical distribution function

The Wigner distribution function $\rho(q, p, t)$ satisfies the equation [5]

$$\frac{\partial\rho}{\partial t} + \frac{p}{m}\frac{\partial\rho}{\partial q} + \int K(q, p - p')\rho(q, p', t)\,\mathrm{d}p' = 0 \tag{2.1}$$

where (q, p) is a point in phase space and the kernel K is given by

$$K(q, p-p') = \frac{\mathrm{i}}{\hbar}\int \frac{\mathrm{d}v}{2\pi\hbar}\exp\left[\frac{\mathrm{i}}{\hbar}(p-p')v\right]\left[V\left(q-\frac{v}{2}\right) - V\left(q+\frac{v}{2}\right)\right] \tag{2.2}$$

where $V(q)$ is the potential. In the classical limit [5] equation (2.2) becomes

$$\begin{aligned} K_c(q, p-p') &= -\frac{\mathrm{i}}{\hbar}\int \frac{\mathrm{d}v}{2\pi\hbar}\exp\left[\frac{\mathrm{i}}{\hbar}(p-p')v\right] v\frac{\partial V}{\partial q} \\ &= -\frac{\partial V}{\partial q}\frac{\partial}{\partial p}\delta(p-p'). \end{aligned} \tag{2.3}$$

and equation (2.1) goes over into the Liouville equation

$$\frac{\partial \rho_c}{\partial t} + \frac{p}{m}\frac{\partial \rho_c}{\partial q} - \frac{\partial V}{\partial q}\frac{\partial \rho_c}{\partial p} = 0. \tag{2.4}$$

The problem we are addressing is to find the particular solution ρ_c of (2.4), which may be considered the correct semiclassical approximation of a given solution ρ of (2.1). One may relate ρ and ρ_c, for instance, by assuming that at time $t = t_0$ both distributions coincide and that afterwards they evolve following (2.1) and (2.4), respectively. The classical path of a particle subject to the potential $V(q)$ which at time $t = 0$ occupies the phase-space point (q_0, p_0) will be denoted by

$$q = Q(q_0, p_0, t) \qquad p = P(q_0, p_0, t) \tag{2.5}$$

so that

$$q_0 = Q(q_0, p_0, 0) \qquad p_0 = P(q_0, p_0, 0). \tag{2.6}$$

Then the CDF, ρ_c which at time t_0 coincides with the WDF ρ, will be given by [6]

$$\rho_c(q, p, t) = \rho(Q(q, p, t_0 - t), P(q, p, t_0 - t), t_0). \tag{2.7}$$

However, this mapping is not unique due to the arbitrariness of t_0. In addition, for stationary ρ, the function ρ_c will, in general, not be stationary, a property which ought to be preserved in the semiclassical approximation. However, in the case of scattering, one may derive an appropriate mapping from (2.7). Consider $\rho(q, p, t)$ as the WDF which corresponds to the scattering solution of the Schrödinger equation such that one has an incident plane wave at time $t = t_0$. By making t_0 recede to $-\infty$, ρ as well as ρ_c (given by (2.7)) will become stationary. This CDF was introduced by Lee and Scully [3] and describes classical scattering.

In order to derive the proposed mapping we introduce the retarded Green's function $G_c(q, p; q', p', t - t')$, which satisfies the inhomogeneous Liouville equation [1]

$$\frac{\partial G_c}{\partial t} + \frac{p}{m}\frac{\partial G_c}{\partial q} - \frac{\partial V}{\partial q}\frac{\partial G_c}{\partial p} = \delta(q-q')\delta(p-p')\delta(t-t'). \tag{2.8}$$

With the help of G_c we write the following integral equation relating ρ and ρ_c [1]:

$$\begin{aligned} \rho(q, p, t) = \rho_c(q, p, t) &- \int_{-\infty}^{\infty}\mathrm{d}t' \int \mathrm{d}q'\,\mathrm{d}p'\, G_c(q, p; q', p', t-t') \\ &\times \int \mathrm{d}p''\left[K(q', p'-p'') - K_c(q', p'-p'')\right]\rho(q', p'', t'). \end{aligned} \tag{2.9}$$

If a WDF ρ satisfying (2.1) is inserted into (2.9), the resulting function ρ_c can be shown to satisfy (2.4). Thus, equation (2.9) may, in principle, generate a CDF from a known WDF, and we shall use it as a starting point of our prescription for the determination of ρ_c. Here let us make the remark that, conversely, for a ρ_c satisfying (2.1), equation (2.9) does not, in general, yield a solution ρ corresponding to a quantum mechanically pure state. In many cases the integral on the right-hand side of (2.9) does not converge as it stands and, in order to obtain definite results, a convergence factor has to be introduced. We shall utilize the usual factor $\exp(\epsilon t')$, the limit $\epsilon \to 0_+$ is taken after the integration over time in (2.9) has been performed [7].

The WDF generated by a given wavefunction $\psi(q, t)$ is [8]

$$\rho(p, q, t) = \int \frac{\mathrm{d}v}{2\pi\hbar} \exp\left(\frac{ipv}{\hbar}\right) \psi\left(q - \frac{v}{2}, t\right) \psi^*\left(q + \frac{v}{2}, t\right). \tag{2.10}$$

Here we shall mainly be interested in the case in which ψ is stationary and thus ρ does not depend on the time. Next we shall try to rewrite (2.9) in a more manageable form. Either by expressing ρ in terms of ψ through its definition (2.10), and by applying the Schrödinger equation subsequently, or by directly using (2.1) and (2.3); equation (2.9) may be written

$$\begin{aligned}\rho_c(q, p, t) = \rho(q, p, t) + \int_{-\infty}^{+\infty} \mathrm{d}t' \int \mathrm{d}q'\, \mathrm{d}p' G_c(q, p; q', p', t - t') \\ \times \left[-\frac{\partial}{\partial t'} - \frac{p'}{m}\frac{\partial}{\partial q'} + \frac{\partial V}{\partial q'}\frac{\partial}{\partial p'} \right] \rho(q', p', t').\end{aligned} \tag{2.11}$$

Equation (2.11) is equivalent to (2.9) provided ρ satisfies (2.1). We make the remark here that in the particular case in which $V(q)$ is quadratic in q, equation (2.11) reduces to the equation $\rho = \rho_c$, as in this case (2.1) becomes identical to the Liouville equation, so that the integrand in (2.11) vanishes. The retarded Green's function (solution of (2.8)) is known to be

$$G_c(q, p; q', p', \tau, \epsilon) = \mathrm{e}^{-\epsilon\tau} \delta(Q(q, p, -\tau) - q') \delta(P(q, p, -\tau) - p') \eta_+(\tau) \tag{2.12}$$

where Q and P are defined by (2.5) and (2.6), η_+ is the step function and where, in addition, we introduced the convergence factor explicitly. Inserting G_c from (2.12) into (2.11) we get

$$\begin{aligned}\rho_c(q, p, t) = \rho(q, p, t) - \int_{-\infty}^{t} \mathrm{d}t' \exp(-\epsilon(t - t')) \\ \times \left[\left(\frac{\partial}{\partial t'} + \frac{p'}{m}\frac{\partial}{\partial q'} - \frac{\partial V}{\partial q'}\frac{\partial}{\partial p'} \right) \rho(q', p', t') \right]_{q'=Q(q,p,t'-t),\, p'=P(q,p,t'-t)}.\end{aligned} \tag{2.13}$$

The above expression may be further simplified by using the classical equations of motion

$$\frac{P}{m} = \frac{\partial}{\partial t'} Q(q, p, t' - t) \qquad -\frac{\partial V}{\partial Q} = \frac{\partial}{\partial t'} P(q, p, t' - t) \tag{2.14}$$

from which we get

$$\begin{aligned}\left[\left(\frac{\partial}{\partial t'} + \frac{p'}{m}\frac{\partial}{\partial q'} - \frac{\partial V}{\partial q'}\frac{\partial}{\partial p'} \right) \rho(q', p', t') \right]_{q'=Q(q,p,t'-t),\, p'=P(q,p,t'-t)} \\ = \frac{\partial}{\partial t'} \rho(Q(q, p, t' - t), P(q, p, t' - t), t')\end{aligned} \tag{2.15}$$

and equation (2.13) becomes

$$\rho_c(q, p, t) = \rho(q, p, t) - \int_{-\infty}^{t} \mathrm{d}t' \exp(-\epsilon(t - t')) \frac{\partial}{\partial t'} \rho(Q(q, p, t' - t), P(q, p, t' - t, t')) \tag{2.16}$$

where $\rho_c(q,p,t)$ is seen to be independent of time provided $\rho(q,p,t)$ does not depend on it. In those cases in which ϵ may be set equal to zero from the beginning we get from (2.16)

$$\rho_c(q,p,t) = \lim_{t'\to-\infty} \rho(Q(q,p,t'), P(q,p,t'), t') . \tag{2.17}$$

This expression gives us back the mapping defined previously through (2.7), in the special case in which the initial time t_0 is set equal to $-\infty$. Thus, if the limit defined by (2.17) does exist the value of ρ_c at the phase-space point (q,p) is the value assumed by ρ at the initial ($t = -\infty$) phase-space point of the classical trajectory, which at time $t = 0$ does pass through the point (q,p). In what follows we shall assume that ρ does not depend on the time. Returning to (2.16), introducing $\tau = t' - t$ as a new variable of integration and performing an integration by parts we get for our mapping equation

$$\rho_c(q,p) = \lim_{\epsilon\to0_+} \epsilon \int_{-\infty}^{0} \mathrm{d}\tau\, \exp(\epsilon\tau)\rho(Q(q,p,\tau), P(q,p,\tau)) . \tag{2.18}$$

In the derivation of (2.18) we made use of condition (2.6).

We now consider the special case in which the point (q,p) belongs to a closed classical path. This happens for a system of one degree of freedom at phase-space points where the energy $E(q,p)$ is negative. In this case (2.17) is not applicable and we use (2.18). Let us perform the Fourier decomposition

$$\rho(Q(q,p,\tau), P(q,p,\tau)) = \sum_{n=-\infty}^{\infty} R_n(q,p)\mathrm{e}^{\mathrm{i}n\omega(q,p)\tau} \tag{2.19}$$

where $T(q,p) = 2\pi/\omega(q,p)$ is the period associated with the trajectory. Inserting the expansion (2.19) into (2.18) we obtain that the only non-vanishing contribution in the $\epsilon = 0_+$ limit arises from the $n = 0$ term of the series (2.19). Thus we get

$$\rho_c(q,p) = R_0(q,p) = (T(q,p))^{-1} \int_0^{T(q,p)} \mathrm{d}\tau\, \rho(Q(q,p,\tau), P(q,p,\tau)) . \tag{2.20}$$

For points on the same closed path (2.20) gives the same value of ρ_c as the trajectories associated with these points are connected to each other by making time translations and (2.20) is invariant under time translations.

This last result can be seen to be valid in general. Thus, for two points (q,p) and (q',p') on the same path, consider the time interval $\Delta\tau$ needed to go from one point to the other, that is, such that

$$Q(q',p',\tau) = Q(q,p,\tau+\Delta\tau) \qquad P(q',p',\tau) = P(q,p,\tau+\Delta\tau) . \tag{2.21}$$

From equation (2.18), by making $\tau = \tau' + \Delta\tau$ we get

$$\begin{aligned}\rho_c(q,p) &= \lim_{\epsilon\to0_+} \epsilon \int_{-\infty}^{-\Delta\tau} \mathrm{d}\tau'\, \mathrm{e}^{\epsilon(\tau'+\Delta\tau)} \rho(Q(q',p',\tau'), P(q',p',\tau')) \\ &= \rho_c(q',p') + \lim_{\epsilon\to0_+} \epsilon \int_0^{-\Delta\tau} \mathrm{d}\tau'\, \mathrm{e}^{\epsilon(\tau'+\Delta\tau)} \rho(Q(q',p',\tau'), P(q',p',\tau')) \\ &= \rho_c(q',p')\end{aligned} \tag{2.22}$$

since the term with the finite integration interval $\Delta\tau$ vanishes, so that $\rho_c(q,p)$ will be constant along any trajectory, and hence a constant of motion. From this fact alone one concludes that ρ_c satisfies the time-independent Liouville equation. Thus, by taking the total derivative of ρ_c with respect to the time, one gets

$$\frac{\mathrm{d}\rho_c}{\mathrm{d}t} = \dot{q}\frac{\partial\rho_c}{\partial p} + \dot{p}\frac{\partial\rho_c}{\partial p} = \frac{\partial E}{\partial p}\frac{\partial\rho_c}{\partial q} - \frac{\partial E}{\partial q}\frac{\partial\rho_c}{\partial p} = 0 . \tag{2.23}$$

Inserting $E(q, p) = p^2/2m + V(q)$ one obtains the Liouville equation.

Let us now discuss the important case of the WDF corresponding to a bound state in a potential which vanishes at infinity. For bound states it is known that $\rho(q, p)$ vanishes asymptotically as $|q|$ tends to infinity. Since the trajectories having positive energy are not bounded but start at $|q| = +\infty$ at time $t = -\infty$, equation (2.17) may be applied directly, the result being that $\rho_c(q, p) = 0$ for points with positive energy $E(q, p)$. Thus the mapped CDF may be viewed in this case as a stationary distribution function of classical particles trapped by the potential.

It may be worthwhile pointing out that in the case of one degree of freedom the value of the CDF at a point (q_0, p_0) corresponding to negative energies $E_0 = E(q_0, p_0)$, may also be obtained by taking the average of the corresponding WDF over the strip $S(q_0, p_0, \delta E)$ defined by the points in phase space possessing an energy in the interval $(E_0 - \frac{\delta E}{2}, E_0 + \frac{\delta E}{2})$, δE being an infinitesimal. In order to derive this result, consider for each energy E in the strip $S(q_0, p_0, \delta E)$ a classical trajectory $(Q(E, t), P(E, t))$, $0 \leqslant t \leqslant T(E)$, $T(E)$ being its period. Thus we get a one-to-one correspondence between the pairs (E, t) and the points (q, p) inside the strip. Consider the integral

$$\int_{E_0-\frac{\delta E}{2}}^{E_0+\frac{\delta E}{2}} \mathrm{d}E\,(T(E))^{-1} \int_0^{T(E)} \mathrm{d}t\, \rho(Q(E,t), P(E,t))$$

$$= \int_{E_0-\frac{\delta E}{2}}^{E_0+\frac{\delta E}{2}} \mathrm{d}E\, \rho_c(Q(E,0), P(E,0)) \approx \delta E\, \rho_c(q_0, p_0) \tag{2.24}$$

where we used (2.20) for ρ_c and the fact that ρ_c is constant along the classical paths. Now make the transformation of variables [9]

$$q = Q(E,t) \qquad p = P(E,t) \qquad 0 \leqslant t \leqslant T(E) \tag{2.25}$$

for the points on the strip. Then the volume element in phase space transforms according to $\mathrm{d}E\,\mathrm{d}t = |J|\,\mathrm{d}q\,\mathrm{d}p$, where the Jacobian J is given by

$$J^{-1} = \begin{vmatrix} \frac{\partial p}{\partial E} & \frac{\partial q}{\partial E} \\ \frac{\partial p}{\partial t} & \frac{\partial q}{\partial t} \end{vmatrix} = \frac{\partial p}{\partial E}\frac{\partial E}{\partial p} + \frac{\partial q}{\partial E}\frac{\partial E}{\partial q} = 1 \tag{2.26}$$

where we used Hamilton's equations of motion. Thus an alternative expression for ρ_c in the case of one degree of freedom is

$$\rho_c(q, p) = \lim_{\delta E \to 0} \int_{S(q,p,\delta E)} \rho(q', p')\,\mathrm{d}q'\,\mathrm{d}p' \left(\int_{S(q,p,\delta E)} \mathrm{d}q'\,\mathrm{d}p' \right)^{-1}. \tag{2.27}$$

3. The infinite square well

As an example of a CDF generated by a WDF corresponding to a bound-state wavefunction we shall consider the ground state of the infinite square well

$$V(q) = \begin{cases} 0 & |q| \leqslant a \\ \infty & |q| > a. \end{cases} \tag{3.1}$$

The wavefunction is

$$\psi(q) = \sqrt{\frac{2}{a}} \cos\frac{\pi q}{2a} \qquad |q| \leqslant a \tag{3.2}$$

and the corresponding WDF [10] is given by

$$\rho(Q,P) = \frac{1}{2\pi\hbar a}\left\{\frac{\hbar}{2P}\left[\sin\left(\frac{2P}{\hbar}(a-Q)+\frac{\pi}{a}Q\right)+\sin\left(\frac{2P}{\hbar}(a-Q)-\frac{\pi}{a}Q\right)\right]\right.$$
$$+\left(\frac{2P}{\hbar}+\frac{\pi}{a}\right)^{-1}\sin\left[\left(\frac{2P}{\hbar}+\frac{\pi}{a}\right)(a-Q)\right]$$
$$\left.+\left(\frac{2P}{\hbar}-\frac{\pi}{a}\right)^{-1}\sin\left[\left(\frac{2P}{\hbar}-\frac{\pi}{a}\right)(a-Q)\right]\right\} \qquad Q>0 \tag{3.3}$$

$$\rho(Q,P)=\rho(-Q,P) \qquad Q<0\,. \tag{3.4}$$

The density ρ can also be seen to be symmetric under the exchange of P by $-P$. The trajectory which starts at time $t=0$ at position $q=-a$ and momentum p ($p>0$) is given by

$$\begin{aligned} Q(-a,p,t) &= \frac{p}{m}t-a \qquad P(-a,p,t)=p \qquad 0\leqslant t\leqslant\frac{2am}{p} \\ Q(-a,p,t) &= \frac{p}{m}t+3a \qquad P(-a,p,t)=-p \qquad \frac{2am}{p}\leqslant t\leqslant\frac{4am}{p}\,. \end{aligned} \tag{3.5}$$

Following equation (2.20) we find for the CDF

$$\rho_c(-a,p)=\frac{1}{T}\left\{\int_0^{\frac{T}{2}}\rho\left(\frac{p}{m}t-a,p\right)\mathrm{d}t+\int_{\frac{T}{2}}^{T}\rho\left(-\frac{p}{m}t+3a,-p\right)\mathrm{d}t\right\} \qquad p>0 \tag{3.6}$$

where $T=4am/p$ is the period of motion of the particle in the box. Making the change of variables $q'=pt/m-a$ in the first integral of (3.6) and $q'=-pt/m+3a$ in the second, one gets

$$\rho_c(-a,p)=\frac{1}{4a}\int_{-a}^{a}\rho(q',p)\,\mathrm{d}q'+\frac{1}{4a}\int_{-a}^{a}\rho(q',-p)\,\mathrm{d}q'\,. \tag{3.7}$$

As the classical trajectory does pass through all coordinate points inside the box without change of momentum, we obtain for an arbitrary point in phase space

$$\rho_c(q,p)=\frac{1}{2a}\int_{-a}^{a}\rho(q',p)\,\mathrm{d}q'=\frac{\pi}{4\hbar}\left[\left(\frac{\pi}{2}\right)^2-\left(\frac{ap}{\hbar}\right)^2\right]^{-2}\cos^2\left(\frac{pa}{\hbar}\right)\,. \tag{3.8}$$

It should be mentioned that in this example ρ_c coincides with the quantum mechanical probability density in momentum space. We remark here that the result (3.7) may also be derived from (2.27). In the limit $\hbar\to 0$ equation (3.8) gives $\rho_c(q,p)\to(2a)^{-1}\delta(p)$ which describes a uniform distribution of particles at rest inside the box, that is, classically the particle is at rest in the ground state.

4. The potential step

As a second example let us consider the potential step

$$V(q)=\begin{cases}0 & q<0\\ V_0>0 & q\geqslant 0\end{cases} \tag{4.1}$$

for incident energies $E = k^2/2m < V_0$. The wavefunction is written

$$\psi(q) = \begin{cases} 2A\cos\left(\frac{kq}{\hbar} - \frac{\alpha}{2}\right) & q < 0 \\ 2A\cos\left(\frac{\alpha}{2}\right)\exp\left(-\frac{\kappa q}{\hbar}\right) & q > 0 \end{cases} \tag{4.2}$$

where

$$\kappa = (2mV_0 - k^2)^{\frac{1}{2}} \tag{4.3}$$

and the phase α is given by

$$\exp(\mathrm{i}\alpha) = \frac{\mathrm{i}k + \kappa}{\mathrm{i}k - \kappa}. \tag{4.4}$$

The WDF in the half-space $Q < 0$, is given by [10]

$$\rho(Q,P) = 4\frac{|A|^2}{\pi}\left\{C^{(-)}(P,k)\cos\left(2(P-k)\frac{Q}{\hbar}\right) + C^{(+)}(P,k)\cos\left(2(P+k)\frac{Q}{\hbar}\right)\right.$$
$$\left. + S^{(-)}(P,k)\sin\left(2(P-k)\frac{Q}{\hbar}\right) + S^{(+)}(P,k)\sin\left(2(P+k)\frac{Q}{\hbar}\right)\right\} \tag{4.5}$$

where

$$C^{(\mp)}(P,k) = \kappa k[(\mp 2P + k)^2 + \kappa^2]^{-1}(\pm 2P)^{-1} \tag{4.6}$$

$$S^{(\mp)}(P,k) = \frac{k(\pm 2Pk - k^2 + \kappa^2)}{[(\mp 2P + k)^2 + \kappa^2]4P(k \mp P)}. \tag{4.7}$$

If $Q > 0$,we have

$$\rho(Q,P) = \frac{4|A|^2}{\pi}\exp(-2\kappa Q)\left\{C_0(P,k)\cos\left(\frac{2PQ}{\hbar}\right) + S_0(P,k)\sin\left(\frac{2PQ}{\hbar}\right)\right\} \tag{4.8}$$

$$C_0(P,k) = 4\kappa k^2[(2P+k)^2 + \kappa^2]^{-1}[(2P-k)^2 + \kappa^2]^{-1} \tag{4.9}$$

$$S_0(P,k) = \frac{k^2(k^2 + \kappa^2 - 4P^2)}{[(2P+k)^2 + \kappa^2][(2P-k)^2 + \kappa^2]P}. \tag{4.10}$$

As can be verified from the above equation, the WDF is a symmetric function under the exchange of P by $-P$.

In the calculation of the CDF we divide the phase space into the five sectors (i)–(v) as follows.

(i) *Subspace ($q < 0$, $p > 0$).* In this subspace the classical trajectories satisfying the condition (2.6) are the straight lines

$$Q(q,p,t) = q + \frac{p}{m}t \qquad P(q,p,t) = p \qquad t < 0 \tag{4.11}$$

since no potential acts during this time. Inserting equation (4.11) into (4.5), we find that the evaluation of (2.18) for ρ_c requires the following integrals:

$$\lim_{\epsilon\to 0}\epsilon\int_{-\infty}^{0}\mathrm{d}t\,\mathrm{e}^{\epsilon t}\cos(\alpha t) = \lim_{\epsilon\to 0}\frac{\epsilon^2}{\epsilon^2+\alpha^2} = \begin{cases} 0 & \alpha \neq 0 \\ 1 & \alpha = 0 \end{cases} \tag{4.12}$$

$$\lim_{\epsilon\to 0}\epsilon\int_{-\infty}^{0}\mathrm{d}t\,\mathrm{e}^{\epsilon t}\sin(\alpha t) = \lim_{\epsilon\to 0}\frac{\epsilon\alpha}{\epsilon^2+\alpha^2} = -\alpha\delta(\alpha)\pi\,. \tag{4.13}$$

By making the indicated substitutions we get, disregarding the integrals (4.12) which give vanishing contributions,

$$\begin{aligned}\rho_c(q,p) = 4|A|^2\{&C^{(-)}(p,k)\sin(2\beta^{(-)}q)(2\beta^{(-)}p)\delta(2\beta^{(-)}p)\\ &+C^{(+)}(p,k)\sin(2\beta^{(+)}q)(2\beta^{(+)}p)\delta(2\beta^{(+)}p)\\ &-S^{(-)}(p,k)\cos(2\beta^{(-)}q)(2\beta^{(-)}p)\delta(2\beta^{(-)}p)\\ &-S^{(+)}(p,k)\cos(2\beta^{(+)}q)(2\beta^{(+)}p)\delta(2\beta^{(+)}p)\}\end{aligned} \tag{4.14}$$

where

$$\beta^{(+)} = \frac{p}{\hbar} + \frac{k}{\hbar} \qquad \beta^{(-)} = \frac{p}{\hbar} - \frac{k}{\hbar}\,. \tag{4.15}$$

Taking account of the delta functions in (4.14) ρ_c will be non-vanishing only at the momenta values $p = k$ and $p = 0_+$. With regard to $p = k$, the only contributing term in (4.14) is the term proportional to $S^{(-)}(p,k)$ because this function has a pole at $p = k$. Thus we find by inserting (4.7) into (4.14)

$$\rho_c(q,p) = |A|^2\delta(p-k) \qquad q < 0 \qquad p > 0\,. \tag{4.16}$$

At the value $p = 0_+$ of the momentum, we obtain that ρ_c vanishes because of cancellations of the various contributions of (4.14). It should be observed that for equilibrium points ($p = 0, \partial V/\partial q = 0$), ρ_c does not need to be continuous, as in this case the classical trajectory shrinks to a single point.

(ii) *Subspace* ($q < 0$, $-\sqrt{2mV_0} < p < 0$). The trajectory which passes through a point (q,p) in this subspace also passes through the point $(q,-p)$ at an earlier time, because of reflection from the barrier at $q = 0$. As ρ_c is a constant of motion we get for the points in sector (ii),

$$\rho_c(q,p) = \rho_c(q,-p) = |A|^2\delta(p+k)\,. \tag{4.17}$$

(iii) *Subspace* ($q > 0$, $p > 0$). From the fact that any trajectory that passes at time $t = 0$ through a given point (q,p) in subspace (iii) does pass also through the point $(-q, \sqrt{p^2+2mV_0})$ in sector (i) at an earlier time, we get from (4.16) the result

$$\rho_c(q,p) = \rho_c(-q,\sqrt{p^2+2mV_0}) = |A|^2\delta(\sqrt{p^2+2mV_0}-k)\,. \tag{4.18}$$

Since we are assuming $k^2 < 2mV_0$, we have $\rho_c = 0$ in this subspace.

(iv) *Subspace* ($q > 0$, $p < 0$). The trajectories which at time $t = 0$ reach the points of this subspace start at $q = +\infty$ at time $t = -\infty$. Since $\rho(q,p) \to 0$ as $q \to +\infty$ we may use (2.17), concluding that ρ_c vanishes in the sector (iv) of the phase space

(v) *Subspace* ($q < 0$, $p < -\sqrt{2mV_0}$). The same reasoning used for region (iv) shows that ρ_c also vanishes in this sector.

We thus come to the conclusion that the CDF which corresponds to the WDF given by (4.5) and (4.8) is

$$\rho_c(q,p) = \begin{cases} |A|^2(\delta(p-k)+\delta(p+k)) & q < 0 \\ 0 & q > 0\,. \end{cases} \tag{4.19}$$

Equation (4.19) describes the reflection of a classical particle subject to the potential (4.1) for energies below the height of the barrier. Similarly, for incident energies above the barrier one finds that no particles will be reflected. These results may be generalized to scattering by a combination of square wells.

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