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January/95

IFT-P.001/95

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Classical Distribution Functions derived from Wigner Distribution Functions

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December 8, 1994

PACS 03.65.Sq

Abstract : A mapping which relates the Wigner phase-space distribution function associated with a given stationary quantum-mechanical wave function 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 wave function, 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 satisfies already 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 consider only 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, one expects to obtain essentially 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]

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

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

$$K(q, p - p') = \frac{i}{h} \int \frac{dv}{2\pi h} \exp \left[\frac{i}{h} (p - p') v \right] \left[V \left(q - \frac{v}{2} \right) - V \left(q + \frac{v}{2} \right) \right], \quad (2.2)$$

$V(q)$ being the potential. In the classical limit [5] eq.(2.2) becomes

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

and eq.(2.1) goes over into the Liouville equation

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

The problem we are addressing is to find that particular solution ρ_c of eq.(2.4) which may be considered the correct semiclassical approximation of a given solution ρ of eq.(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 eqs.(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

$$q = Q(q_0, p_0, t), \quad p = P(q_0, p_0, t), \quad (2.5)$$

so that

$$q_0 = Q(q_0, p_0, 0), \quad p_0 = P(q_0, p_0, 0). \quad (2.6)$$

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

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

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 eq.(2.7). Consider $\rho(q, p, t)$ 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 eq.(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]

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

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

$$\begin{aligned} \rho(q, p, t) &= \rho_c(q, p, t) - \int_{-\infty}^{\infty} dt' \int dq' dp' G_c(q, p; q', p', t - t') \\ &\quad \times \int dp'' [K(q', p' - p'') - K_c(q', p' - p'')] \rho(q', p'', t'). \end{aligned} \quad (2.9)$$

If a WDF ρ satisfying eq.(2.1) is inserted into eq.(2.9) the function ρ_c which comes out can be shown to satisfy eq.(2.4). Thus eq.(2.9) may in principle generate a CDF from a known WDF, and we shall use it as starting point of our prescription for the determination of ρ_c . Let us here make the remark that, conversely, for a ρ_c satisfying eq.(2.1), eq.(2.9) does not yield, in general, a solution ρ corresponding to a quantum mechanically pure state. In many cases the integral on the right hand side of eq.(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 $\epsilon \rightarrow 0_+$ is taken after the integration in the time in eq.(2.9) has been performed [7].

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

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

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

$$\rho_c(q, p, t) = \rho(q, p, t) + \int_{-\infty}^{+\infty} dt' \int dq' dp' G_c(q, p; q', p', t - t') \times \left[-\frac{\partial}{\partial t'} - \frac{p'}{m} \frac{\partial}{\partial q'} + \frac{\partial V}{\partial q'} \frac{\partial}{\partial p'} \right] \rho(q', p', t'). \quad (2.11)$$

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

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

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

$$\rho_c(q, p, t) = \rho(q, p, t) - \int_{-\infty}^t dt' \exp(-\epsilon(t - t')) \left[\left(\frac{\partial}{\partial t'} + \frac{p'}{m} \frac{\partial}{\partial q'} - \frac{\partial V}{\partial q'} \frac{\partial}{\partial p'} \right) \rho(q', p', t') \right]_{q'=Q(q, p, t'-t), p'=P(q, p, t'-t)} \quad (2.13)$$

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

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

from which we get

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

and eq.(2.13) becomes

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

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 eq.(2.16)

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

This expression gives us back the mapping defined previously through eq.(2.7), in the special case in which the initial time t_0 is set equal to $-\infty$. Thus if the limit defined by eq.(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 eq.(2.16), introducing $\tau = t' - t$ as new variable of integration and performing an integration by parts we get for our mapping equation

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

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

We consider now 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 eq.(2.17) is not applicable and we use eq.(2.18). Let us perform the Fourier decomposition

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

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

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

For points on the same closed path the expression (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 eq.(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

$$Q(q', p', \tau) = Q(q, p, \tau + \Delta\tau), \quad P(q', p', \tau) = P(q, p, \tau + \Delta\tau). \quad (2.21)$$

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

$$\begin{aligned} \rho_c(q, p) &= \lim_{\epsilon \rightarrow 0^+} \epsilon \int_{-\infty}^{-\Delta\tau} d\tau' e^{\epsilon(\tau' + \Delta\tau)} \rho(Q(q', p', \tau'), P(q', p', \tau')) \\ &= \rho_c(q', p') + \lim_{\epsilon \rightarrow 0^+} \epsilon \int_0^{-\Delta\tau} d\tau' e^{\epsilon(\tau' + \Delta\tau)} \rho(Q(q', p', \tau'), P(q', p', \tau')) \\ &= \rho_c(q', p'), \end{aligned} \quad (2.22)$$

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

$$\frac{d\rho_c}{dt} = q \frac{\partial \rho_c}{\partial p} + p \frac{\partial \rho_c}{\partial q} = \frac{\partial E}{\partial p} \frac{\partial \rho_c}{\partial q} - \frac{\partial E}{\partial q} \frac{\partial \rho_c}{\partial p} = 0. \quad (2.23)$$

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

Let us discuss now 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 $t = -\infty$, eq.(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 to point 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 be also 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 $(Q(E, t), P(E, t))$, $0 \leq t \leq T(E)$, $T(E)$ 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

$$\begin{aligned} &\int_{E_0 - \frac{\delta E}{2}}^{E_0 + \frac{\delta E}{2}} dE (T(E))^{-1} \int_0^{T(E)} dt \rho(Q(E, t), P(E, t)) \\ &= \int_{E_0 - \frac{\delta E}{2}}^{E_0 + \frac{\delta E}{2}} dE \rho_c(Q(E, 0), P(E, 0)) \approx \delta E \rho_c(q_0, p_0), \end{aligned} \quad (2.24)$$

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

$$q = Q(E, t), \quad p = P(E, t), \quad 0 \leq t \leq T(E), \quad (2.25)$$

for the points on the strip. Then the volume element in phase-space transforms according to $dE dt = |J| dq dp$, where the Jacobian J is given by

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

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

$$\rho_c(q, p) = \lim_{\delta E \rightarrow 0} \int_{S(q, p, \delta E)} \rho(q', p') dq' dp' \left(\int_{S(q, p, \delta E)} dq' dp' \right)^{-1} \quad (2.27)$$

3 The Infinite Square Well

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

$$V(q) = \begin{cases} 0 & |q| \leq a \\ \infty & |q| > a \end{cases} \quad (3.1)$$

The wave function is

$$\psi(q) = \sqrt{\frac{2}{a}} \cos \frac{\pi q}{2a}, |q| \leq a \quad (3.2)$$

and the corresponding WDF [10] is given by

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

$$\rho(Q, P) = \rho(-Q, P), Q < 0. \quad (3.4)$$

The density ρ can be seen to be symmetric also 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

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

Following eq.(2.20) we get for the CDF

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

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 eq.(3.6) and $q' = -pt/m + 3a$ in the

second, one gets

$$\rho_c(-a, p) = \frac{1}{4a} \int_{-a}^a \rho(q', p) dq' + \frac{1}{4a} \int_{-a}^a \rho(q', -p) dq', \quad (3.7)$$

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

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

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 be derived from eq.(2.27) also. In the limit $\hbar \rightarrow 0$ eq.(3.8) gives $\rho_c(q, p) \rightarrow (2a)^{-1} \delta(p)$ 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's consider the potential step

$$V(q) = \begin{cases} 0 & , q < 0 \\ V_0 > 0 & , q \geq 0 \end{cases}, \quad (4.1)$$

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

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

where

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

and the phase α is given by

$$\exp(i\alpha) = \frac{ik + \kappa}{ik - \kappa}. \quad (4.4)$$

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

$$\begin{aligned} \rho(Q, P) = & 4 \frac{|A|^2}{\pi} \left\{ C^{(-)}(P, k) \cos\left(2(P-k)\frac{Q}{h}\right) + C^{(+)}(P, k) \cos\left(2(P+k)\frac{Q}{h}\right) \right. \\ & \left. + S^{(-)}(P, k) \sin\left(2(P-k)\frac{Q}{h}\right) + S^{(+)}(P, k) \sin\left(2(P+k)\frac{Q}{h}\right) \right\}, \end{aligned} \quad (4.5)$$

where .

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

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

If $Q > 0$, we have

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

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

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

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

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

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

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

$$\lim_{\epsilon \rightarrow 0} \epsilon \int_{-\infty}^0 dt e^{\epsilon t} \sin(\alpha t) = \lim_{\epsilon \rightarrow 0} \frac{\epsilon \alpha}{\epsilon^2 + \alpha^2} = -\alpha \delta(\alpha) \pi. \quad (4.13)$$

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

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

where

$$\beta^{(+)} = \frac{p}{h} + \frac{k}{h}, \quad \beta^{(-)} = \frac{p}{h} - \frac{k}{h}. \quad (4.15)$$

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

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

At the value $p = 0_+$ of the momentum, we obtain that ρ_c vanishes because of cancellations of the various contributions of eq.(ref4.14). 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 does pass 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 the sector (II),

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

(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 Eq. (4.16) the result

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

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 $\rho(q, p) \rightarrow 0$ as $q \rightarrow +\infty$ 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 vanishes also in this sector.

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

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

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 obtains that no particles will be reflected. These results may be generalized to scattering by a combination of square wells.

References

[1] V. I. Tatarskii, Sov. Phys. Usp. 26, 311, 1983;

[2] Y. L. Shirokov, Teor. Math. Phys. (USSR) 31, 488, 1983;

[3] H. W. Lee and M. O. Scully, J. Chem. Phys. 75, 1048, 1981;

[4] H. W. Lee and M. O. Scully, J. Chem. Phys. 77, 4604, 1982;

[5] P. Carruthers and F. Zachariasen, Rev. Mod. Phys. 55, 245, 1983;

[6] D. N. Zubarev, Non equilibrium Statistical Thermodynamics, pg. 8, Consultants Bureau, Plenum, New York - London, 1974;

[7] J. Stone, Phys. Rev. A26, 1157, 1982;

[8] E. Wigner, Phys. Rev. 40, 719, 1932;

[9] D. H. Kobe, Am. J. Phys. 61, 1031, 1993;

[10] H. W. Lee and M. O. Scully, Found. of Phys. 13, 61, 1983