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Time-dependent quantum tunnelling via crossover processes

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Abstract. It is shown that the propagator $K(xt|x'0)$ for a particle in a potential field is derivable from the classical path starting from x' and reaching x at time t. Considering a wavepacket as the particle initial state lying mainly on one side of a barrier the propagator is used for obtaining the wavefunction on the other side. Tunnelling is then discussed in terms of the evolving wavefunction. It is argued that while the particle's expectation energy is taken to be lower than the barrier height the transformation by which the wavefunction is produced entails energetically crossover flights as required by the dynamics for the classical paths involved in the propagation process. The parabolic repeller exemplifies the formalism and exact results for the probability and current densities are given. A computation involving ballistic tunnelling shows that the current density rises to a saturation value proportional to the particles' injection rate.

1. Introduction

In the customary treatment of the phenomenon of quantum tunnelling one relies on obtaining an approximate solution of the Schrödinger equation relating to a potential barrier within the WKB scheme for energies below the barrier height. Such a solution extends all over space and so the probability of finding the particle even in regions classically prohibited on account of insufficient energy does exist.

Here we shall be taking a different point of view, outlined in the case of one-dimensional motion. We consider a particle in the field of a potential barrier in a state initially prepared in the form of a wavepacket

$$\Phi_{(x_0,p_0)}(x) = (2\pi\sigma^2)^{-1/4} \exp\left(-\frac{1}{4\sigma^2}(x-x_0)^2 + \frac{i}{\hbar} p_0 x\right). \tag{1.1}$$

Such a wavepacket locates the particle at the phase point (x_0, p_0) with minimum uncertainty irrespective of the variance σ^2. With appropriate choice of the variance the probability of finding the particle can be appreciable in a narrow region around x_0. However, the particle's energy expectation value may on certain occasions be dependent on σ^2, a situation that places a limit on the smallness of the variance if we wish the energy expectation value to be smaller than the barrier height.

The state (1.1) establishes a certain initial probability distribution of finding the particle in a region around the point x_0, which throughout this work will be assumed to be on the LHS of the barrier. Thus a portion, the most significant part of the probability distribution, lies mainly on the LHS of the barrier and, furthermore, the distribution may extend through a tail on the other side. Our approach to the tunnelling problem will rely on processes leading to transport of the above initial probability

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from the LHS to the RHS of the barrier. Contrary to the situation expected from classical thinking there occurs a flow of probability from left to right even when the particle's expectation energy is smaller than the barrier height, a state of affairs that characterises the tunnelling effect.

When the potential energy associated with the barrier is independent of time the particle's expected energy is a constant of the motion. This constant is taken against the evolving wavefunction yielding the transformed probability distribution producing the tunnelling effect. The linear transformation, as we shall show subsequently, can be constructed from a single classical path joining an initial spacetime point $(x', 0)$ with the spacetime point (x, t) labelling the wavefunction at position x and time t. This path, being classical, is associated with the right amount of energy as required by classical dynamics. Therefore, whenever in the process of transformation of the initial wavefunction in the course of time x' and x happen to be on different sides of the barrier the transformation is effected through a crossover procedure, i.e. a procedure requiring the classical amount of energy to overcome the barrier in the specified time t. The shorter the time of flight the higher the amount of energy required and definitely in excess of the barrier height. We summarise as follows. In the tunnelling effect, while the energy associated with the wavefunction is lower than the barrier height, the propagation of the wavefunction in time is effected through a set of appropriate flight processes for which the classical energy requirement is fulfilled. This picture of the tunnelling phenomenon constitutes one of the main results of the paper.

Let us now proceed by putting things in a more concrete fashion. Beginning with an initial state described by the wavepacket (1.1) we can find the solution of the Schrödinger equation associated with the barrier potential energy by propagating the initial state. Thus, if $K(xt|x'0)$ is the system's propagator the required solution has the form

$$\Psi_{(x_0,p_0)}(x, t) = \int K(xt|x'0)\Phi_{(x_0,p_0)}(x')\, \mathrm{d}x'. \tag{1.2}$$

Once the evolving wavefunction (1.2) is known the probability of finding the particle in a region on the RHS of the barrier as a function of time is known. Furthermore, the evolution of the current density at some point x on the RHS of the barrier can be found through the usual formula as

$$j(x, t) = \mathrm{Re}\,\frac{\hbar}{mi}\,\Psi^*_{(x_0,p_0)}(x, t)\,\frac{\partial}{\partial x}\,\Psi_{(x_0,p_0)}(x, t). \tag{1.3}$$

It is clear that the scheme outlined above is based on the propagator associated with the barrier problem.

For the purpose of gaining insight into the tunnelling problem we proceed in section 2 in a way that allows us to build our propagator by extending the semiclassical propagator. This also enables us to make contact with the WKB procedure employed in the time independent approach, and furthermore we can draw certain comparisons particularly in relation to the use of the energy parameter appearing in both schemes. In this section we further show that the exact quantum mechanical propagator $K(xt|x'0)$ can be obtained from just a single classical path $X_c(\tau)$, namely the path satisfying the end conditions $X_c(0) = x'$ and $X_c(t) = x$. This is a result of general validity revealing an interesting aspect of quantum dynamical theory.

Section 3 exploits the structure of the propagator in terms of the classical path $X_c(\tau) = X_c(xt|x'0; \tau)$, satisfying the classical equation of motion and joining the spacetime points $(x', 0)$ and (x, t), for obtaining a formula for the current density at a point x (observation point) at time t. It is seen that the current density can be cast as a linear superposition of quantities involving the classical momentum $P_c(xt|x'0)$ and a corresponding purely quantal momentum $P_q(xt|x'0)$ joining the point $(x', 0)$ as an initial spacetime point and a final one (x, t) with x the observation point and t the corresponding time. The superposition is taken against the initial wavefunction and the propagator over all initial points x'. In the final analysis the current density evolves via a flight process described by the classical path $X_c(xt|x'0; \tau)$. The energy associated with this path is in accordance with the classical dynamical requirements. Thus, when x' and x are on different sides of the barrier the energy involved pertains to a crossover state of affairs. In contrast, the expectation energy value associated with the initial state can be smaller than the barrier height, which means that the current density at the observation point is of tunnelling origin.

Furthermore, this section accommodates the notion of the transmission coefficient as a ratio of two probabilities B/A, A being the probability of finding the particle initially on the LHS of the barrier and B the net probability that it has migrated onto the other side after a very long time.

Section 4 illustrates the preceding approach to the tunnelling problem using as a vehicle the parabolic repeller. This is an interesting situation in that there are no periodic bound states. Exact results are presented for the probability and current densities. The probability density is a drifting Gaussian about the classical path determined by the initial phase space point (x_0, p_0) entering the wavepacket (1.1). The current density involves two terms, one relating to the classical momentum $P(t)$ associated with the path that goes through the initial phase space point (x_0, p_0) and the Hamilton classical momentum $P_c(xt|x'0)$ associated with the path which joins the spacetime points $(x_0, 0)$ and (x, t). A not so common situation is shown to emerge when p_0, the initial particle momentum, points in the negative direction. In this case $P(t)$ is negative since the particle is pushed away towards $-\infty$, whereas $P_c(xt|x_0 0)$ is positive. There is then an interplay between P and P_c, as a result of which we get initially a negative current at the observation point which after a while becomes positive. This is an interesting aspect in that, although the probability density centre recedes from the barrier, a current develops in the opposite direction on the other side of the barrier.

Finally, our approach provides a natural frame for the handling of ballistic tunnelling. Ballistic tunnelling is treated in the case of the parabolic repeller and it is seen that the current density reaches a saturation value which is proportional to the entry frequency.

2. The propagator

It has been shown by Van Vleck [1] that the semiclassical propagator for potential energy $U(x)$ takes the form

$$K_c(xt|x'0) = \left(\frac{D(xt|x'0)}{2\pi i\hbar}\right)^{1/2} \exp\left(\frac{i}{\hbar} S_c(xt|x'0)\right) \tag{2.1}$$

where $S_c(xt|x'0)$ is the classical action associated with the particle's motion under the specification that at time $t = 0$ the particle is at x' and goes through x at time t, and

D for the one-dimensional case is given by

$$D(xt\,|\,x'0) = -\frac{\partial^2}{\partial x\,\partial x'} S_c(xt\,|\,x'0). \tag{2.2}$$

Furthermore, it has been shown by Pauli [2] that K_c satisfies the essential initial condition

$$K_c(xt\,|\,x'0) \to \delta(x - x') \qquad \text{as } t \to 0 \tag{2.3}$$

required by the full quantal propagator $K(xt\,|\,x'0)$. In addition Dirac [3] has shown, without using the form (2.2), that D satisfies the continuity equation.

Before seeking a more accurate expression for the quantal propagator we wish to digress somewhat in order to draw certain comparisons with the customarily employed time-independent form of the WKB approximation.

We begin with the Hamilton-Jacobi equation

$$-\frac{\partial S}{\partial t} = \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + U(x) \tag{2.4}$$

from which the classical action S_c in (2.1) can be derived.

It is well known that the expression

$$S = \int_{x'}^{x} \pm\sqrt{2m(E - U(\xi))}\,\mathrm{d}\xi - Et \tag{2.5}$$

satisfies (2.4) for any value of the arbitrary constant E. In a way S in (2.5) is a general solution of (2.4).

However, we are interested in the solution containing the necessary information about the classical path $X_c(\tau)$ depicting the particle's motion specified by the end conditions $X_c(0) = x'$ and $X_c(t) = x$. Under these circumstances E (the system's energy) is of course a constant of the motion, but depends on the end conditions i.e. $E = E(xt\,|\,x'0)$ and is determined by the additional equation

$$\partial S/\partial E = 0 \tag{2.6}$$

which expresses the fact that the energy is fixed by the time t taken by our particle to move from x' to x in the field of force produced by the given potential. The expression for $E = E(xt\,|\,x'0)$ determined through (2.6) when introduced into (2.5) leads to the required classical action $S_c(xt\,|\,x'0)$ used in (2.1).

In contrast, in the customary application of the WKB approximation the energy, E, appears as if it were an arbitrary parameter. This leads to a situation in which the author experiences difficulty in obtaining a reconciliation between the complete arbitrariness of the energy constant of motion as employed in the time-independent WKB approximation and the restriction on this constant deriving from its dependence on the end spacetime conditions in the semiclassical treatment of the propagator.

Let us now improve on the propagator beyond the semiclassical stage. To this end we write the full quantal propagator in the form

$$K(xt\,|\,x'0) = K_c(xt\,|\,x'0)\exp\left(\frac{\mathrm{i}}{\hbar} Q(xt\,|\,x'0)\right). \tag{2.7}$$

On combining (2.1) with (2.7) the resulting exponential argument becomes $S_c + Q$ and this is what might be called the quantal action, at least for reasons of communication in the text. Q is the purely quantal part of the action.

Upon introducing (2.7) into the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right)K \tag{2.8}$$

the following equation for the motion of the purely quantal part of the action, Q, is obtained:

$$\frac{\partial Q}{\partial t}+\frac{1}{m}\frac{\partial S_c}{\partial x}\frac{\partial Q}{\partial x}=-\frac{1}{2m}\left(\frac{\partial Q}{\partial x}\right)^2+\frac{i\hbar}{2m}\frac{\partial^2 Q}{\partial x^2}+\frac{1}{2m}\left[\hbar^2\left(\frac{1}{2D}\frac{\partial D}{\partial x}\right)^2+i\hbar\frac{1}{D}\frac{\partial D}{\partial x}\frac{\partial Q}{\partial x}\right]. \tag{2.9}$$

Equation (2.9) governs the motion of the purely quantal part of the system's action. On account of the initial condition (2.3) satisfied by K_c and the fact that the same initial condition is required of the complete quantal propagator, we are led from (2.7) that the constraint

$$Q(xt\,|\,x'0)\rightarrow 0 \qquad \text{as } t\rightarrow 0 \tag{2.10}$$

is placed as the initial condition on Q.

Let us now proceed to solve (2.9) as a power series in $\hbar$. On inspection the lowest power in $\hbar$ for which there is a non-zero solution is 2. So we write

$$Q=\sum_{n=2}^{\infty}\hbar^n Q_n. \tag{2.11}$$

Introducing (2.11) into (2.9) and equating on both sides the terms of same power in $\hbar$ we obtain the following hierarchy of equations:

$$\left(\frac{\partial}{\partial t}+\frac{1}{m}\frac{\partial S_c}{\partial x}\frac{\partial}{\partial x}\right)Q_n=F_n(xt\,|\,x'0) \qquad n=2,3,\ldots \tag{2.12}$$

where the double argument function F_n is made out of the various $\partial Q_j/\partial x$ ($j=2,\ldots,n-1$).

The first few F_n are given below and a general formula becomes established for $n>4$:

$$F_2=\frac{1}{8m}\left(\frac{1}{D}\frac{\partial D}{\partial x}\right)^2 \tag{2.13a}$$

$$F_3=\frac{i}{2m}\left(\frac{1}{D}\frac{\partial D}{\partial x}\frac{\partial Q_2}{\partial x}+\frac{\partial^2 Q_2}{\partial x^2}\right) \tag{2.13b}$$

$$F_4=\frac{i}{2m}\left(\frac{1}{D}\frac{\partial D}{\partial x}\frac{\partial Q_3}{\partial x}+\frac{\partial^2 Q_3}{\partial x^2}\right)-\frac{1}{2m}\left(\frac{\partial Q_2}{\partial x}\right)^2 \tag{2.13c}$$

and for $n\geqslant 4$ we have

$$F_n=\frac{i}{2m}\left(\frac{1}{D}\frac{\partial D}{\partial x}\frac{\partial Q_{n-1}}{\partial x}+\frac{\partial^2 Q_{n-1}}{\partial x^2}\right)-\frac{1}{2m}\sum_{j+k=n}\frac{\partial Q_j}{\partial x}\frac{\partial Q_k}{\partial x}. \tag{2.13d}$$

We now proceed to show that the hierarchy of equations (2.12) can be solved once the classical path $X_c(\tau)$ followed by the particle in the field of force dictated by the potential energy $U(x)$ and satisfying the end conditions $X_c(0)=x'$ and $X_c(t)=x$ is available. For this path we make use of the notation

$$X_c(\tau)=X_c(xt\,|\,x'0;\,\tau) \tag{2.14}$$

indicating the end conditions which it incorporates. In fact knowledge of the path (2.14) leads to the classical action S_c through the formula

$$S_c(xt|x'0)=\int_0^t\left(\frac{m}{2}\dot{X}_c^2(\tau)-U(X_c(\tau))\right)\mathrm{d}\tau \qquad (2.15)$$

and furthermore D is obtained via (2.2). D supplies F_2 via (2.13a) and from (2.12) Q_2 is made known. This enables F_3 to be obtained and therefore Q_3 and so on. There remains to show how (2.14) for the classical path leads to the required solutions of (2.12).

For solving (2.12) we proceed to obtain the propagator of the corresponding homogeneous equation

$$\frac{\partial Q}{\partial t}+\frac{1}{m}\frac{\partial S_c}{\partial x}\frac{\partial Q}{\partial x}=0. \qquad (2.16)$$

Clearly the coefficient of $\partial Q/\partial x$ in (2.16) is the classical velocity which the particle will have at time t in its motion through the potential field U, provided at time $t=0$ it is at x' and goes through x at time t. Utilising a revealing notation we write

$$V_c(xt|x'0)=\frac{1}{m}\frac{\partial}{\partial x}S_c(xt|x'0). \qquad (2.17)$$

We proceed to establish the relation

$$\frac{\partial}{\partial t}X_c(xt|x'0;\tau)=-V_c(xt|x'0)\frac{\partial}{\partial x}X_c(xt|x'0;\tau). \qquad (2.18)$$

This is so, since the particle coordinate at time τ determined by the path that passes through the spacetime points $(x'0)$ and (x,t) will not change by varying t and x on the original path. Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t}X_c(\tau)=\frac{\partial}{\partial t}X_c(\tau)+\frac{\mathrm{d}x}{\mathrm{d}t}\frac{\partial}{\partial x}X_c(\tau)=0. \qquad (2.19)$$

On taking account of the fact that

$$\frac{\mathrm{d}x}{\mathrm{d}t}=V_c(xt|x'0) \qquad (2.20)$$

we establish (2.18).

Let us now construct the conditional deterministic probability distribution of finding our particle at time τ in the vicinity of ξ with the proviso that the spacetime particle trajectory passes through $(x',0)$ and (x,t). We have

$$G(xt|x'0;\xi\tau)=\delta(X_c(xt|x'0;\tau)-\xi). \qquad (2.21)$$

Introducing G from (2.21) into (2.16) in place of Q and taking account of (2.17) and (2.18) we find that (2.16) is satisfied. Furthermore, (2.21) fulfils the initial condition

$$G(xt|x'0;\xi\tau)\to\delta(x-\xi) \qquad \text{as } \tau\to t. \qquad (2.22)$$

So, G is the propagator of (2.16) and incorporates the end conditions of our path.

With the aid of (2.21) we can write the solution for the hierarchy of equations (2.12) as

$$Q_n(xt|x'0)=\int_0^t\mathrm{d}\tau\int\mathrm{d}\xi\,G(xt|x'0;\xi\tau)F_n(\xi\tau|x'0) \qquad n=2,3,\ldots \qquad (2.23)$$

The Q_n given by (2.23) not only satisfy the equations of the hierarchy, but also fulfil the right initial condition (2.10).

Utilising (2.21) we can write (2.23) as

$$Q_n(xt|x'0) = \int_0^t \mathrm{d}\tau\, F_n(X_c(xt|x'0;\,\tau)\tau|x'0) \qquad n = 2, 3, \ldots. \tag{2.24}$$

The preceding evaluations show that the classical path $X_c(xt|x'0;\,\tau)$ is the only quantity needed for obtaining the quantal propagator. Thus, we reach the remarkable conclusion that the whole of quantum mechanics can be derived from just a single classical path, namely the one passing through two specified spacetime points.

3. Tunnelling as a superposition of crossover processes

In the previous section we have shown how one can obtain the full quantal propagator $K(xt|x'0)$ for a particle in a potential field $U(x)$ from a single classical path, namely the path $X_c(\tau) = X_c(xt|x'0;\,\tau)$ joining the spacetime points $(x', 0)$ and (x, t). It should be noted that obtaining this path in an analytic form in general is not an easy task. However, in cases where the potential energy is such that does not allow the existence of a complete set (or possibly any at all) of periodic energy eigenfunctions the method utilising the above classical path for the propagator becomes particularly useful. The situation in tunnelling problems involves this sort of potential energy where extensive repulsive regions are present.

We shall use as a vehicle for our presentation the case where the potential energy involves a repulsive hump and the initial state of our particle will be described by a wavepacket of the form (1.1) locating it at a point x_0 (expected position) on the LHS of the barrier. Furthermore, the expectation value of the particle's energy will be smaller than the barrier height, so that classically the particle will be unable to find itself on the other side of the barrier on account of insufficient energy. The probability and current densities will be obtained at a point x on the RHS of the barrier. For the sake of communication we shall refer to the points x_0 and x as entry and observation position respectively.

The probability density at the observation point x at time t corresponding to an entry at position x_0 at $t = 0$ is obtained from the square modulus of (1.2) as

$$\rho(x, t) = \frac{1}{2\pi\hbar} \left| \int [D(xt|x'0)]^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar}[S_c(xt|x'0) + Q(xt|x'0)]\right\} \times \Phi_{(x_0,p_0)}(x')\,\mathrm{d}x' \right|^2 \tag{3.1}$$

where in (3.1) we have made use of (2.7) for the propagator.

The essential feature in the tunnelling effect lies in that part of the probability of finding the particle initially on the entry side of the barrier moves into the observation side. The ratio of the net amount of probability on the RHS of the barrier that has migrated into this region in time t over the initial probability of finding the particle on the entry side is given by

$$T(t) = \left[\int_{-\infty}^{x_m} \rho(x, 0)\,\mathrm{d}x\right]^{-1} \int_{x_m}^{\infty} [\rho(x, t) - \rho(x, 0)]\,\mathrm{d}x \tag{3.2}$$

where x_m is the coordinate of the barrier top.

The transmission coefficient in this frame is obtained from $T(t)$ in the limit of $t \to \infty$, and the reflection coefficient by $R = 1 - T$, giving the ratio of the probability of finding the particle on the entry side after a long time (remainder of probability) over the corresponding initial probability.

The definition made for the transmission coefficient through (3.2) embodies the essential feature of transmission for it gives the 'portion of the particle that moved onto the other side of the barrier' after a long time. However, it applies well only in the case where the potential maximum is located at a single point x_m. The situation where the potential has a flat maximum requires modification. The fact that x_m appears in the process of obtaining the transmission coefficient serves only for an implicit introduction of the barrier height $U_m = U(x_m)$, a quantity appearing in this coefficient when one employs the usual asymptotic procedure for its evaluation.

In section 2 we have seen that the propagator $K(xt|x'0)$ can be generated entirely from the classical path $X_c(xt|x'0;\, \tau)$. This path represents a flight process from the point x' to the point x in time t and is consistent with the classical energy requirement. This means that the energy associated with the flight (a constant of motion) is greater than the particle's maximum potential energy occurring between x' and x. The shorter the flight time the larger the energy associated with the path.

With the above in mind let us consider the case for which the initial state (1.1) locates the particle sufficiently far away from the coordinate of the barrier top in an adequately narrow region so that the wavefunction extends initially on the RHS of the barrier, at most, through an insignificant tail. Under these circumstances the probability of finding the particle on the entry side differs negligibly from unity. Having stated the situation for the initial state $\Phi_{(x_0,p_0)}(x)$ the required information about the tunnelling process at the observation point x is obtained from the wavefunction $\Psi_{(x_0,p_0)}(x, t)$ via (1.2) as a superposition of the propagator $K(xt|x'0)$ against the initial state $\Phi_{(x_0,p_0)}(x')$ over all x', essentially lying on the entry side. Clearly, this superposition for the making of $\Psi_{(x_0,p_0)}(x, t)$ utilises, through the processes involved in the propagator, all classical flights from x' to x in time t with x' belonging to the region where the initial wavefunction is significant and which is located on the entry side. As has been pointed out earlier the energy required for each flight corresponds to a crossover process in contrast to a penetration state of affairs.

In case the probability distribution extends with its tail on the RHS of the barrier the above picture is not invalidated for the bulk of the initial wavefunction, but one has, in addition, to discuss an interference term coming from the propagation of the portions of the initial wavefunction lying on the LHS and the RHS of the barrier.

Next, for the current density at the observation point we utilise (1.3). Combining (1.2), (2.1) and (1.3) we have

$$j(x, t) = \mathrm{Re}\, \frac{1}{m} \Psi^*_{(x_0,p_0)}(x, t) \int \left(\frac{i\hbar}{2D(xt|x'0)} \frac{\partial^2}{\partial x\, \partial x'} P_c(xt|x'0) + P_c(xt|x'0) + P_q(xt|x'0) \right) K(xt|x'0)\Phi_{(x_0,p_0)}(x')\, dx' \tag{3.3}$$

where P_q is the purely quantum counterpart of the classical momentum P_c, and is given by

$$P_q(xt|x'0) = \frac{\partial}{\partial x} Q(xt|x'0). \tag{3.4}$$

In case the potential energy is a polynomial at most quadratic in x the first term in the square brackets on the RHS of (3.3) is zero, and so is the purely quantum momentum P_q. In such a case the semiclassical propagator coincides with the exact quantal propagator, and the current density is obtained as a superposition of the classical momenta $P_c(xt|x'0)$ over the initial positions x' in the region where the initial wavepacket extends.

In general P_q is non-zero as well as the derivatives of P_c appearing in (3.3). In addition to the propagator the quantities P_q and P_c and the latter's derivatives are obtained from the classical path $X_c(xt|x'0;\tau)$ which, as stated earlier, is consistent with the energy required by the particle to overcome the barrier in its crossover flight from x' to x in time t. The decomposition of the probability and current densities, according to (3.1) and (3.3), in terms of crossover processes regarding the making of the propagator and the various momenta is the main result of this section. However, as pointed out earlier in the tunnelling effect, the initial wavepacket is associated with an expectation energy below the one required for a classical crossover process.

The next section deals with a simple application of formulae (3.1) and (3.3) for which we can obtain exact results, and thus the foregoing discussion is elucidated through a concrete example.

4. Tunnelling through the parabolic repeller

A situation where the above formalism can be exemplified in an exact fashion is the parabolic repeller. The potential energy under consideration is given by

$$U(x) = -\tfrac{1}{2}m\Omega^2x^2. \tag{4.1}$$

Although this is a relatively simple case it is instructive in that it presents itself as an instance where the system has no periodic energy eigenstates at all. Furthermore, one cannot consider, with ease, as an initial state a plane wave of considerable extension since it is difficult to prepare such a state in an increasingly repulsive field of force. In contrast, when a particle comes out of a source its state is essentially localised and a wavepacket in the form (1.1) can be well suited to describing the particle's initial state.

Employing Newton's equation of motion for a particle with potential energy (4.1) we find that the path passing through the spacetime points $(x', 0)$ and (x, t) is given by

$$X_c(xt|x'0;\tau) = x'(\cosh\Omega\tau - \coth\Omega t\sinh\Omega\tau) + x\frac{\sinh\Omega\tau}{\sinh\Omega t}. \tag{4.2}$$

Introducing $X_c(\tau) = X_c(xt|x'0;\tau)$ from (4.2) in (2.15) we obtain the associated classical action as

$$S_c(xt|x'0) = \frac{m\Omega}{2\sinh\Omega t}[(x^2+x'^2)\cosh\Omega t - 2xx']. \tag{4.3}$$

Furthermore, the double argument function D obtained from (2.2) is given by

$$D(xt|x'0) = \frac{m\Omega}{\sinh\Omega t}. \tag{4.4}$$

Since D is independent of spatial coordinates the hierarchy of equations (2.12) together with the initial condition yield that the purely quantum action is in this case zero. Thus, the semiclassical propagator provides the exact propagator.

Upon application of (1.2) we find the wavefunction at the observation point x at time t as

$$\Psi_{(x_0,p_0)}(x, t) = (2\pi\sigma^2)^{-1/4}\Gamma(t)^{-1/2} \exp\left(\frac{\mathrm{i}}{\hbar} S_c(xt\,|\,x_0 0)\right)$$

$$\times \exp\left(-\frac{\mathrm{i}m\Omega}{2\hbar \sinh \Omega t}(x - X(t))^2 + \frac{\mathrm{i}}{\hbar} p_0 x_0\right) \tag{4.5}$$

where

$$X(t) = x_0 \cosh \Omega t + \frac{p_0}{m} \sinh \Omega t \tag{4.6}$$

$$\Gamma(t) = \cosh \Omega t + \mathrm{i}\frac{\hbar}{2m\Omega\sigma^2} \sinh \Omega t. \tag{4.7}$$

$X(t)$ in (4.6) is the position reached by the classical particle at time t if it started at x_0 with momentum p_0. In general $X(\tau)$, specified through the phase space point (x_0, p_0) as initial condition defines a different classical path from the path $X_c(\tau) = X_c(xt\,|\,x_0 0;\, \tau)$ specified through the end conditions $(x_0, 0)$ and (x, t). For the latter path we have used the subscript c. In order that the paths $X(\tau)$ and $X_c(\tau)$ coincide the initial momentum appearing in $X(\tau)$ must be chosen in such a way so that $X(t) = x$ is satisfied.

Expression (4.5) for the evolution of the wavepacket (1.1) is in accord with the result obtained earlier [4] by an alternative method, and the probability density of finding the particle in the vicinity of the observation point x at time t is given by

$$\rho_{(x,t)} = (2\pi\sigma^2|\Gamma(t)|^2)^{-1/2} \exp\left(-\frac{(x - X(t))^2}{2\sigma^2|\Gamma(t)|^2}\right) \tag{4.8}$$

where $|\Gamma(t)|^2$ can be obtained from (4.7) as

$$|\Gamma(t)|^2 = \cosh^2 \Omega t + \left(\frac{\lambda}{\sigma}\right)^4 \sinh^2 \Omega t \tag{4.9}$$

where in (4.9) we have introduced

$$\lambda = (\hbar/2m\Omega)^{1/2} \tag{4.10}$$

which is a characteristic length of the scattering processes associated with the potential energy (4.1).

Utilising (1.3) or (3.3) in relation to (4.1) we obtain the current density at the observation points x at time t as

$$j(x, t) = \frac{1}{m|\Gamma(t)|^2}\{P(t) + [1 + (\lambda/\sigma)^4] \sinh^2 \Omega t\, P_c(xt\,|\,x_0 0)\}\rho(x, t) \tag{4.11}$$

where $P(t)$ is the particle's classical momentum under the initial condtions $X(0) = x_0$, $P(0) = p_0$ and is given by

$$P'(t) = p_0 \cosh \Omega t + m\Omega x_0 \sinh \Omega t \tag{4.12}$$

and

$$P_c(xt\,|\,x_0 0) = \frac{m\Omega}{\sinh \Omega t}(x \cosh \Omega t - x_0). \tag{4.13}$$

Comparison of (3.3) as applied to the parabolic repeller in which case only the Hamilton momentum $P_c(xt|x'0)$ survives in the square brackets, with (4.11) for the tunnelling current tells us that the superposition of the momenta $P_c(xt|x'0)$ over the region of x' where $\Phi_{(x_0,p_0)}(x')$ extends leads to the appearance of the two classical momenta $P(t)$ and $P_c(xt|x_0 0)$ as contributing factors to the current density. $P(t)$ is the momentum which the particle has at its classical position as determined by the initial phase space conditions (x_0, p_0), whereas $P_c(xt|x_0 0)$ relates only to the starting point x_0 and is the momentum the particle should have at the observation point x if it were to reach this point in time t. When the particle's initial conditions are (x_0, p_0), even for the classical motion the momentum $P_c(xt|x_0 0)$ is some sort of hypothetical momentum.

As explained earlier, the momentum $P_c(xt|x_0 0)$ is consistent with the energy requirement for the particle to crossover the barrier in the specified time. This energy is given by

$$E_c = \frac{m}{2}\Omega^2 \frac{1}{\sinh^2 \Omega t}(x^2 + x_0^2 - 2xx_0 \cosh \Omega t) \tag{4.14}$$

and is constant on the particle's trajectory in spacetime from $(x_0, 0)$ to (x, t).

What actually determines the tunnelling effect is the energy associated with the initial wavepacket, which has to be smaller than the barrier height, as it is determined by the position x_0. Since the system is conservative the expectation value of the particle's energy will remain constant in the course of time. In the present case the expected energy is given by

$$\langle H \rangle = \frac{1}{2m} p_0^2 - \tfrac{1}{2} m\Omega^2 x_0^2 + \tfrac{1}{2} m\Omega^2 \sigma^2 \left(\frac{\lambda^4}{\sigma^4} - 1\right). \tag{4.15}$$

The first two terms on the RHS of (4.15) constitute the particle's classical energy while the last term is an energy produced by the repelling force deforming the wavepacket. This sort of deformation energy depends on the wavepacket's spread expressed by σ^2. If the particle is highly localised (σ^2 very small) the deformation energy is very large and if it is extended (σ^2 large) it becomes negative. When $\lambda = \sigma$ the deformation energy is made equal to zero and so the expected energy equals the classical energy.

In order that the current produced at the observation point be of tunnelling origin we must have $\langle H \rangle < 0$, since the top of the barrier for the potential energy (4.1) is placed at zero. The potential energy at x_0 being $-(1/2m)\Omega^2 x_0^2$, the opposite of which constitutes the energy to be overcome.

Let us now consider a situation in which $\langle H \rangle < 0$ and furthermore $p_0 < 0$, i.e. the particle's classical motion on the RHS of the barrier drives it away from the position of the barrier's top. Thus, $P(t)$ is negative (see (4.12)) while $\sinh^2 \Omega t\, P_c(xt|x_0 0)$ starts from zero and has a positive growth. Under these circumstances the tunnelling current at the observation point will be initially negative and, after a certain time, although the particle classically will be distancing itself from the top of the barrier, a current density will appear at the observation point in the opposite direction. This degree of resolution between the movement of the expected motion of the particle and the building of current on the other side of the barrier has become possible through treating the tunnelling phenomenon in a time-dependent fashion. This situation is more clearly depicted in figure 1.

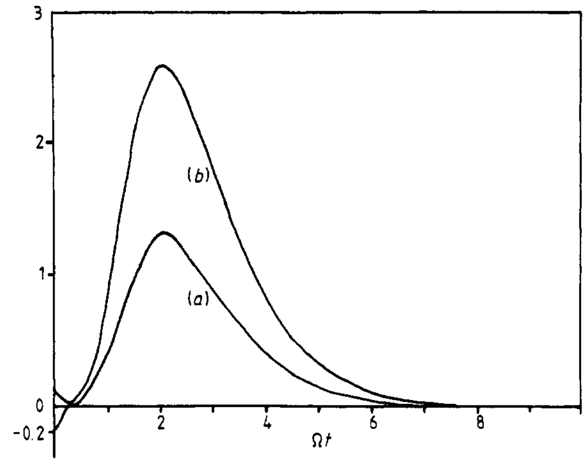

Figure 1. Evolution of probability and current densities for a particle entering the field of the parabolic repeller at $x_0 = -2\lambda$. The particle's expected energy equals the corresponding classical energy, in this case $-7m\Omega^2\lambda^2/8$. Curve (a) is probability density in units of $10^3\ \lambda^{-1}$ and (b) is current density in units of $10^{-3}\Omega$. Although the particle classically moves away from the barrier, after a while a tunnelling current in the opposite direction gets established. The probability density goes down initially and then rises.

A further advantage of the time-dependent formalism lies in that it provides a frame for treating ballistic entry of particles against a barrier [5]. Supposing a situation where particles make their entry, with insufficient energy, at times t_0, t_1, $t_2, \ldots$, then the kth particle generates a tunnelling current $j_k(x, t)$ at the observation point x. Under the above circumstances the total tunnelling current density, J, resulting from the

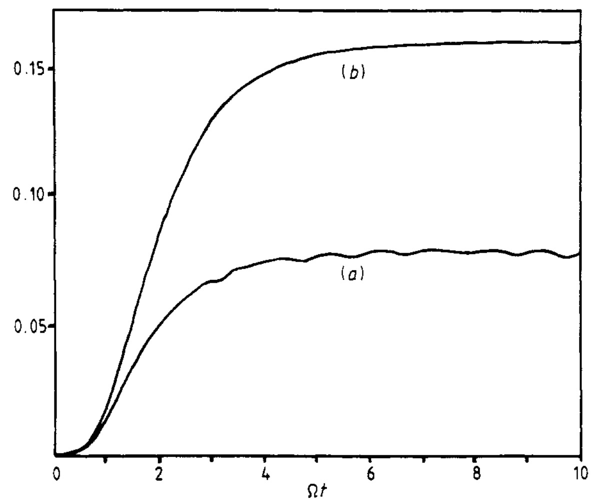

Figure 2. Current density for ballistic tunnelling against a parabolic repeller. Entry of particles at $x_0 = -2\lambda$ at regular intervals with zero speed. Observation at $x = 2\lambda$. The expected energy for each particle equals its classical value which is $-2m\Omega^2\lambda^2$. Curve (a) is entry rate of 1 particle/Ω^{-1} and curve (b) is 2 particles/Ω^{-1}. The current density (units Ω) reaches a saturation value proportional to the entry rate.

stream of particles making their entry at x_0, is given by

$$J(x, t) = \sum_{k=0} j_k(x, t). \tag{4.16}$$

Certain numerical results are presented in figure 2 and show that the ballistic current reaches a saturation value which is proportional to the frequency of the incoming particles.

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