TIME DEPENDENT QUANTUM TUNNELLING

G J Papadopoulos
Department of Physics, Laboratory of Mechanics, University of Athens
Panepistimiopolis GR 157 71 , Zografos Athens-Greece

Abstract
The propagator K(xt | x′o) for a particle in a potential field is shown to be derivable from a single classical path evolving under the field and which at time 0 starts from x′ and reaches x at time t. The wavefunction of a particle represented initially by a wavepacket lying mainly on one side of a barrier is then propagated and supplies information about the particle's probability and current densities on the other side. This approach to tunnelling is seen to be performed via energetically crossover classical flights. Results relating to the parabolic repeller and an eta potential are presencad.

1. Introduction

In a recent paper [1] we have drawn certain comparisons between the customary WKB treatment of the tunnelling phenomenon and the time dependent approach which we adopt here. In this lecture we briefly review the essential points leading to the construction of the quantal propagator from only a single particular classical path. We further enrich the applications, presented here, by the case of an eta potential. In addition we show, through an example, how the principle of superposition can be held responsible for the tunnelling effect.

The discussion for the tunnelling problem will be based on the evolution in time of an initial wavefunction taken to be a wavepacket in the form

$$\Phi_{(x_o,p_o)}(x) = (2\pi\sigma^2)^{-1/4}\exp\left[-\frac{1}{4\sigma^2}(x-x_o)^2 + \frac{i}{\hbar}p_o x\right] \qquad (1.1)$$

which by appropriate choice of x_o lies essentially on the LHS of a barrier which is represented by a potential U(x). At the expectation value level, (1.1) represents a particle at x_o with momentum p_o . In order to restrict ourselves to tunnelling problems the expected energy associated with (1.1) in conjunction with U(x) has to be smaller than the barrier's height. This is attained by an appropriate choice of the parameters x_o, p_o, σ.

The evolving wavefunction on the RHS of the barrier provides all essential information about the tunnelling behaviour of our particle. In this frame we accommodate the notion of transmission coefficient by considering the probability of finding the particle initially on the LHS of the barrier, let it be A, and the probability that at time t the particle has migrated onto the other side of the barrier, let it be B. The transmission coefficient, T , is then given as the ratio B/A. It is in general time dependent and may reach a fixed value after a long time. With this understanting for the transmission coefficient we procceed to see the tunnelling effect in the light of the superposition principle of quantum mechanics. We consider a situation with a single barrier bounded by perfect reflectrors at minus and plus infinities. The requirement of perfect reflectors enables use of periodic eigenfunctions. It is clear that if the state of our system at a given moment is an eigenfunction the probability of finding the particle in a specified region does not change with time and so no tunnelling takes place. Consider, now, the case where the particle's initial state ,$\Psi(x,o)$, is a superposition of , say, two eigenfunctions Φ_1,Φ_2 i.e.

$$\Psi(x,o)= C_1\Phi_1(x) + C_2\Phi_2(x) \tag{1.2}$$

As time proceeds the evolving wavefunction takes the form

$$\Psi(x,t)= C_1\Phi_1(x)\exp(-i\omega_1 t)+ C_2\Phi_2(x)\exp(-i\omega_2 t) \tag{1.3}$$

where ω_1 and ω_2 equal correspondingly $E_1/\hbar$ and $E_2/\hbar$ with E_1,E_2 being the associated energy eigenvalues.

The transmission coefficient at time t pertaining to our situation is given by

$$T(t) =\int_{x_m}^{\infty} [\ |\Psi(x,t)|^2 - |\Psi(x,o)|^2]dx \Big/ \int_{-\infty}^{x_m} |\Psi(x,o)|^2dx \tag{1.4}$$

where x_m is the point at which the potential barrier has its maximum.

The numerator in (1.4) represents the amount of probability B, that has migrated in time t onto the RHS of the barrier. This quantity may be negative, as well, and in the case of the state considered becomes

$$B= 2\{\cos[(\omega_1-\omega_2)t]-1\}\ \mathrm{Re}C_1C_2^*\int_{x_m}^{\infty}\Phi_1\Phi_2^*dx + 2\sin[(\omega_1-\omega_2)t]\ \mathrm{Im}C_1C_2^*\int_{x_m}^{\infty}\Phi_1\Phi_2^*\ dx \tag{1.5}$$

It is the variation with time of the migration probability B that accounts for the tunnelling effect. Note that in our considerations we have not made any assumptions as to the magnitude of the energies E_1,E_2. Both of these energies and, therefore, the expected energy associated with the initial state $\Psi(x,o)$ can be smaller that the barrier's height, and yet produce a nonzero value for T.

2. The propagator

The frame of the time dependent tunnelling is based on following the evolution of a particle's wavefunction that derives from a given initial state. An effective way for obtaining the evolving wavefunction is by use of the associated propagator, which serves as a linear transformation. In what follows we shall sketch how we can obtain the full quantum propagator utilizing a single particular classical path. Our considerations will refer to one dimension, for simplicity, while generalization to many dimensions is straightforward.

We begin with Van Vleck's expression for the semiclassical propagator [2] for a particle whose potential energy is $U(x)$. It has the form

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

where S_c is the classical action, associated with the potential energy $U(x)$, between the space-time points (x',o) and (x,t) and

$$D(xt \mid x'o) = -\frac{\partial^2}{\partial x \partial x'}S_c(xt \mid x'o) \tag{2.2}$$

According to Dirac [3], D obeys a continuity equation.

Although (2.1) satisfies Schrödinger's equation approximately, it does obey, according to Pauli [4], the right initial condition required of the exact propagator, namely

$$K(xt \mid x'o) \longrightarrow \delta(x-x') \quad \text{as} \quad t \longrightarrow 0 \tag{2.3}$$

If we now write the full quantal propagator in the form

$$K(xt \mid x'o) = K_c(xt \mid x'o)\exp\left[\frac{i}{\hbar}Q(xt \mid x'o)\right] \tag{2.4}$$

and employ Schrödinger's equation associated with $U(x)$ we obtain the following equation for the quantity Q which, at least for reasons of communication, we shall call purely quantum action,

$$\frac{\partial Q}{\partial t}+\frac{1}{m}\frac{\partial S_c}{\partial x}\frac{\partial Q}{\partial x} = -\frac{1}{2m}\left(\frac{\partial Q}{\partial x}\right)^2+\frac{i\hbar}{2m}\left[\frac{\partial^2 Q}{\partial x^2}+\frac{1}{D}\frac{\partial D}{\partial x}\frac{\partial Q}{\partial x}\right]+\frac{\hbar^2}{2m}\left[\left(\frac{1}{2D}\frac{\partial D}{\partial x}\right)^2-\frac{1}{2D}\frac{\partial^2 D}{\partial x^2}\right] \tag{2.5}$$

Since K_c satisfies the initial condition required of the propagator K (2.5) must be solved for Q under the initial condition

$$Q(xt \mid x'o) \longrightarrow 0 \quad \text{as } t \longrightarrow 0 \tag{2.6}$$

(2.5) can be solved by iteration. Utilizing an expression for Q in the form

$$Q = \sum_{n=2}^{\infty} \hbar^n Q_n \tag{2.7}$$

we are led to a hierarchy of equations all of which take the form

$$\frac{\partial Q_n}{\partial t} + \frac{1}{m}\frac{\partial S_c}{\partial x}\frac{\partial Q_n}{\partial x} = F_n(xt \mid x'o) \qquad (2.8)$$

with $F_2 = \frac{1}{2m}\left[\left(\frac{1}{2D}\frac{\partial D}{\partial x}\right)^2 - \frac{1}{2D}\frac{\partial^2 D}{\partial x^2}\right]$ known as well as the rest of the F_n's can be made known. Details of the solution can be found in [1] and attention is drawn to a correction made to the term F_2 as above. Here we shall point out certain results.

The solution of (2.8) with the appropriate boundary condition (2.6) can be obtained through the propagator of the equation

$$\frac{\partial Q}{\partial t} + \frac{1}{m}\frac{\partial S_c}{\partial x}\frac{\partial Q}{\partial x} = 0 \qquad (2.9)$$

If $X_c(\tau) = X(xt \mid x'o;\, \tau)$ is the classical path which our system follows form time 0 to t starting form x′ and reaching x then, as has been shown in [1], the required propagator $G(\xi\tau;\, xt \mid x'o)$ is given as

$$G = \delta(\xi - X_c(\tau)) \qquad (2.10)$$

which leads to the required solution of (2.8) as

$$Q_n(xt \mid x'o) = \int_0^t d\tau\, F_n(X_c(\tau)\, \tau \mid x'o) \qquad (2.11)$$

From the above we infer that the quantal propagator can be obtained by use of a single classical path, the path joining the end space-time points of the propagator.

3 Applications

We wish to deal with two cases; namely the parabolic repeller and a case of an eta potential. The first instance, although a simple one, is exaclty soluble and furthermore predicts, contrary to expectations from hitherto experience, a form of negative conductivity. The latter being in the sense that whilst the particle in its classical motion is receding from the potential barrier a tunnelling current may develop on the other side in the opposite direction. The case of an eta potential has interest in that one can study to a certain extent the ecsape through the barrier of a metastable potential for a particle initially trapped in a potential valley.

The parabolic repeller

The parabolic repeller is represented by the potential energy

$$U(x) = -\frac{1}{2}m\Omega x^2 \qquad (3.1)$$

We cite below the expressions for the probability and current densities associated with (3.1), while the reader is refered to [1] for the various steps leading to these expressions. We have

$$\rho(x,t) = \frac{1}{\sqrt{2\pi}\ \sigma\ |\Gamma(t)|} \exp\left[-\frac{(x-X(t))^2}{2\sigma^2\ |\Gamma(t)|^2}\right] \tag{3.2}$$

$$j(x,t) = \frac{1}{m|\Gamma(t)|^2} \{P(t) + [1+(\frac{\lambda}{\sigma})^2]\sinh\Omega t\ P_c(xt \mid x_o o)\}\rho(x,t) \tag{3.3}$$

where X(t) and P(t) are the particle's classical position and momemtum respectively, under the intitial conditions $X(o)=X_o$, $P(o)= p_o$, and are given by

$$X(t)=x_o\cosh\Omega t + \frac{p_o}{m}\sinh\Omega t \tag{3.4}$$

$$P(t) = P_o\ \cosh\Omega t + m\Omega x_0 \sinh\Omega t \tag{3.5}$$

and

$$P_c(xt \mid x_o o) = \frac{m\Omega}{\sinh\Omega t}(x\ \cosh\Omega t - x_o) \tag{3.6}$$

is Hamilton's momentum under the end space-time conditions (x_o,o) and (x,t). λ is a characteristic length associated with the scattering processes induced by the potential (3,1) and is given by

$$\lambda=(\hbar/2m\Omega)^{1/2} \tag{3.7}$$

and finally $\Gamma(t)$ is given by

$$\Gamma(t) = \cosh\Omega t + i(\frac{\lambda}{\sigma})^2\sinh\Omega t \tag{3.8}$$

Figure 1 depicts the appearance of negative conductivity, a situation obtained with p_o negative leading to a classical motion for the wavepacket away from the barrier whilst on the other side the current initially follows the wavepacket's motion but after a while reverses direction.

In figure 2 we have a situation in which particles enter one side of the barrier at intervals in succession and generate a current on the other side; ballistic current

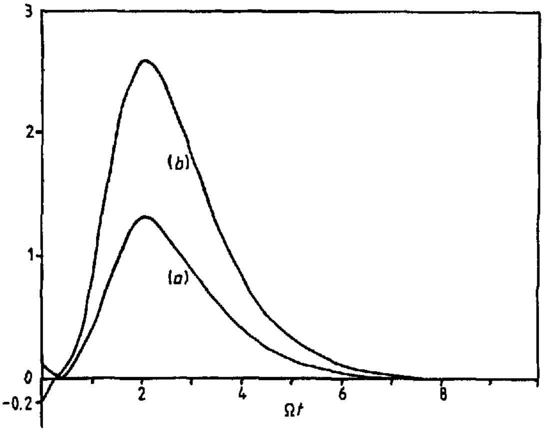

Figure 1. Evolution of probability and current densities for a particle entering the field of the parabolic repeller at $x_0 = -2\lambda$. The particle's expected energy equals the corresponding classical energy, in this case $-7m\Omega^2\lambda^2/8$. Curve (a) is probability density in units of $10^3\,\lambda^{-1}$ 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.

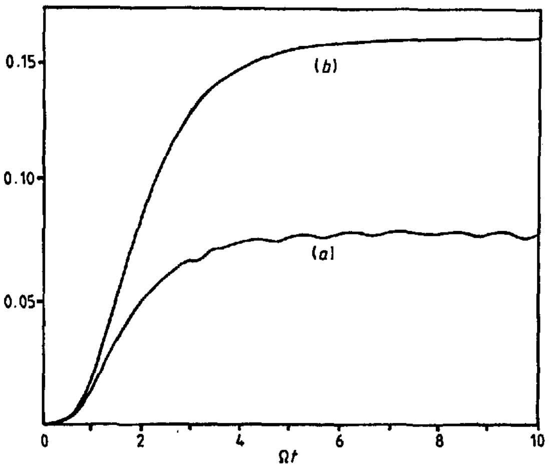

Figure 2. Current density for ballistic tunnelling against a parabolic repeller. Entry of particles at $x_0 = -2\lambda$ at regular intervals with zero speed. Observation at $x = 2\lambda$. The expected energy for each particle equals its classical value which is $-2m\Omega^2\lambda^2$. Curve (a) is 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.

Eta potential

The eta potential we consider here is made out of an oscillator well joint to a parabolic repeller, both appropriately truncated, in the way expressed by the associated potential energy

$$U_e(x)=\begin{cases} \frac{m}{2}\Omega^2x^2 & x \leqslant b/2 \\ \frac{m}{4}\Omega^2b^2 - \frac{m}{2}\Omega(x-b)^2 & x \geqslant b/2 \end{cases} \qquad (3.9)$$

The point at which the two potentials are linked is b/2 and b is the point at which the top of the parabolic repeller portion of the combined potential is located.

For the purpose of studying the tunnelling of a particle, initially trapped in the oscillator valley, through the hump of the repelling portion we require the classical path starting from x' and reaching x in time t with x located on the right of b. If x' is greater than b/2 the situation is straightforward and here we shall restrict ourselves to the case when $x' < b/2$. Denoting by t_m the time at which the particle passes through the matching point b/2 on its way from x', at time 0, to x ,at time t, we have the required path, obtained by Newton's equations, in the form

$$X_c(\tau)=\begin{cases} X_1(\tau) & 0 \leqslant \tau \leqslant t_m \\ X_2(\tau) & t_m \leqslant \tau \leqslant t \end{cases} \qquad (3.10)$$

where

$$X_1(\tau)=x'(\cos\Omega\tau - \cot\Omega t_m \sin\Omega\tau)+ \frac{b}{2}\frac{\sin\Omega\tau}{\sin\Omega t_m} \qquad (3.11)$$

$$X_2(\tau)=b - \frac{b}{2}\;[\cosh\Omega(\tau-t_m)- \coth\Omega(t-t_m)\;\sinh\Omega(\tau-t_m)]+(x-b)\;\frac{\sinh\Omega(\tau-t_m)}{\sinh\Omega(t-t_m)} \qquad (3.12$$

It is clear from (3.11) and (3.12) that at $\tau=t_m$ $X_1(t_m)=X_2(t_m)=b/2$. The matching time t_m is fixed by the continuity requirement that the left and right velocities be equal at the point b/2, i.e.

$$[\frac{d}{d\tau}X_1(\tau)]_{\tau=t_m} =[\frac{d}{d\tau}X_2(\tau)]_{\tau=t_m} \qquad (3.13)$$

Equation (3.13) supplies by computation $t_m=t_m$ (xt I x'o).

The corresponding classical action for the eta potential is obtained by use of the action's additivity property as

$$S_{ce}(xt \mid x'o) = S_2(xt \mid \frac{b}{2}t_m) + S_1(\frac{b}{2}t_m \mid x'o) \qquad (3.14)$$

To obtain S_1 and S_2 is a simple matter and for lack of space their expressions are omitted.

For obtaining the semiclassical propagator we need, in addition to the classical action its derivative $\partial^2 S_{ce} / \partial x\, \partial x'$ .This involves the derivatives of t_m with respect to x and x', which are explicitly obtained as functions of t_m. The semiclassical propagator can now be obtained utilizing (2.1) by inserting the appropriate classical action.

We have employed the above approximate propagator for obtaining the evolution of an initially still wavepacket centred at the bottom of the occillator well valley. The particle's energy was chosen to fulfill the requirement for tunnelling and a numerical evaluation of the evolution of the probability density has been carried out, and shown in figure 3. Reliable results for the probability on the RHS of the barrier have been found for times $t<\pi/2\Omega$. For $t=\pi/2\Omega$ strange things are happening with the classical path; in fact, depending on the initial and final positions, for t very near $\pi/2\Omega$ there may not be a classical flight. Beyond the time $t=\pi/2\Omega$ the situation regularises again.

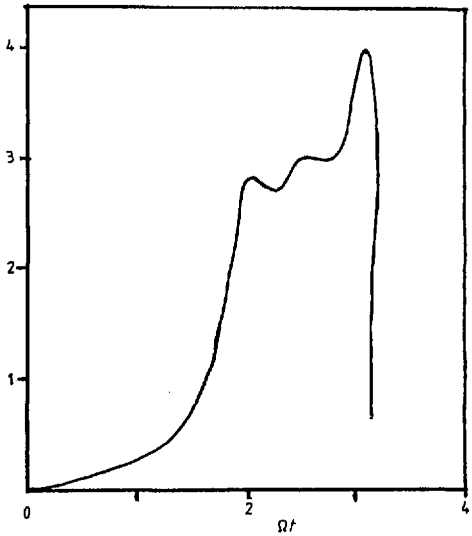

Figure 3. Probability density times 10^3 at x=3b as a function of time. Initial state: still wavepacket centred at well's bottom with energy 2/3 barrier's height.

Acknowledgements

The author should like to thank the organizers, Academician Professor M A Markov, Professor V I Man'ko and Professor V V Dodonov for their invitation to a most enjoyable and profitable Colloquium. He, further, greatfully acknowledges assistance tirelessly rendered by the Man'ko family, Mrs M A Man'ko and daughter O V Man'ko.

References

[1] Papadopoulos G J 1990 Phys. A: Math. Gen. **23** 935-47

[2] Van Vleck J H 1928 Proc. Natl Acad. Sci: USA **14** 178

[3] Dirac P A M 1958 The Principles of Quantum Mechanics (Oxford: Oxford University Press) PP 121-5

[4] Pauli W 1952 Ausgewälte Kapitel der Feldquautisierung (Lecture notes) (Zürich: ETH) pp 139-52