Section 13.1:The Quantum Theory of Motion - Interference and Tunneling*

0.1 Interference

Particle interference is viewed as a characteristic feature of quantum mechanics. An electron beam traversing an optical apparatus such as a two slit arrangement displays, if the appropriate experimental conditions are met, an alternation of bright and dark fringes on a screen placed behind the plane of the slits. This effect is incompatible with the concept of localized point like particles in the classical sense but is qualitatively accounted for by Bohr's idea of wave-particle duality. A physical system exposed to a *wave-like experimental setup* will exhibit wave like behavior. The position-momentum uncertainty relation dispels the cloud of mystery shrouding this statement. Let the incident beam consist of electrons with well-defined momenta, and their positions will be maximally uncertain, resulting in a plane wave description of the incoming particles.

At this point, the historical debate about the completeness of quantum mechanics emerges. Uncertainty forbids assigning simultaneously sharp properties to conjugate observables. Therefore, ensembles in quantum mechanics are radically different from statistical ensembles in classical physics, as the latter involve sets of individual entities specified in terms of conjugate quantities that adopt simultaneously well-defined values. This, however, is the meaning of *ensemble* in the Bohm-de Broglie theory. The proponents of this theory carry the burden of the proof that particle interference distributions can be reproduced within a model based on classical ensembles. Philippides et al. [5] constructed the quantum potential for a two slit particle interference situation, involving an electron beam at an incident energy of 4.5 keV. In this pursuit the path integral method is used to derive the electronic wave function in the space behind the slits. This yields a natural separation between the modulus and the phase factor and thus permits computating the desired quantum potential Q by use of relation (13.6). The cross section through the Q distribution parallel to the plane of the slits, at a well-defined distance behind this plane, exhibits a regular pattern of plateau regions separated by trough lines. Using $\frac{\partial S}{\partial \mathbf{X}} = m\mathbf{V}$ as equation of motion, one generates trajectories determined by the quantum potential. In the trough regions the particles are subjected to strong accelerating forces, acting predominantly in a direction parallel to the plane of the slits and perpendicular to the slit orientation. This causes pronounced kinks in the trajectories which tend to bunch up in the force-free regions of the plateaus, giving rise to the interference structure that is observed in the two-slit experiments involving particles. This result has been obtained employing ensembles of particles that move along classical trajectories, i.e. sequences of individual events. A typical quantum phenomenon has thus been reproduced by virtue of the quantum force as underlying organization scheme.

0.2 Tunneling

The conventional understanding of the tunnel effect has to undergo a thorough revision when examined with the conceptual tools of the quantum theory of motion (QTM). Since this theory operates with the concept of a classical particle on a classical path it must reject the idea of barrier penetration that is at the heart of quantum mechanics. Thus, the challenge of accommodating the tunnel effect, as a cornerstone of quantum theory, within the framework of the Bohm-de Broglie interpretation of quantum phenomena provides a crucial test for its adequacy. Again, the load of reconciling classical thought with experimentally secured quantum effects is carried by the quantum potential. While the potential involved in elementary barrier tunneling problems occurring in quantum mechanics is $V(\mathbf{X})$, i.e. an unchangeable function of the spatial coordinates, the quantum potential changes as the guiding wave propagates. Assuming that it changes such that the effective barrier to be overcome reduces sufficiently upon the approach of the 'tunneling' particle, the concept of barrier penetration could be replaced by the classically admissible one of transmission over the barrier top. Applying the relations (4.54a,b) or their transformed versions (13.17) and (13.19) to tunneling problems makes it possible to study the most essential characteristics of quantum evolution as described in the frame of a causal model.

Pioneering work of Lopreore and Wyatt [9] addressed this issue. The authors defined a density evolution operator to advance the density and construct the quantum potential Q. Subsequently, they solved the equation of motion (13.20) resulting from Q. This *quantum trajectory method* (QTM) was employed in tackling the Eckart barrier problem for a variety of barrier heights and a wide range of translational particle energies E. A one-dimensional situation was assumed, where an ensemble of equally spaced particles was initially arranged around a center X_0 according to the Gaussian distribution $R_0^2(X) = (\frac{2\beta}{\pi})^{1/2} \exp[-2\beta(X - X_0)^2]$. This is the squared modulus of an initial Gaussian wave packet $\Psi_0(X)$:

$$\Psi_0(X) = (\frac{2\beta}{\pi})^{1/4} \exp[-\beta(X - X_0)^2 + ikX] \tag{1}$$

which defines the form of the pilot wave at the starting time. Using Eq.(13.6), one may derive the quantum potential $Q(X)$ from this wave packet. The corresponding *quantum force* results as

$$F_Q = -\frac{dQ(X)}{dX} = \hbar^2 \frac{4\beta^2}{m}(X - X_0) \tag{2}$$

Each particle is endowed with an initial velocity $V = \frac{\hbar K}{m}$, directed towards the Eckart barrier. This implies a uniform kinetic energy for all particles of the incident ensemble. It is, however, crucial for the understanding of the tunnel effect within the Bohm-de Broglie view of quantum mechanics that the kinetic energy is modified *by the action of the quantum force in a non-uniform fashion.*

For further clarification, we refer to the numerical example discussed by Lopreore and Wyatt [9] who included a set of fifty-one particles in their simulation. At the beginning of the motion, the quantum force imparts a boost to those particles with initial positions $X > X_0$, while those with $X < X_0$ experience a decelerating effect. In contrast to the established interpretation of tunneling phenomena, the particles therefore do not approach the barrier with one constant value of the kinetic energy but exhibit a distribution of kinetic energies. This finding eliminates the need for barrier penetration to explain typical manifestations of the tunnel effect. Particles with sufficiently high kinetic energy will skim over the barrier top while those whose kinetic energy falls below the transmission threshold will be reflected.

It is instructive to compare the total force $-\frac{d}{dX}[V(X) + Q(X)]$ involved in this process with the quantum force F_Q. This is done in Figure 13.1 for the first trajectory above and the last trajectory below the transmission threshold (Nos. 27 and 28, respectively), and for an initial translational energy of $E_0 = \frac{3}{4}V_0$, where V_0 denotes the height of the Eckart barrier. For both, the quantum force fades out rapidly as the outer edge of the barrier is reached. During the first 5 fs of the process, however, the quantum force felt along trajectory 28 exceeds markedly that of the competing trajectory. Thus particles moving on the former trajectory pick up a higher amount of kinetic energy during beginning phase of the simulation than those confined to the latter. The total force profiles show that trajectory 28 leads beyond the barrier while 27 is deflected by the barrier.

The observation that the quantum force vanishes during the initial stage of the motion clarifies the mechanism of particle tunneling through potential barriers in terms of the quantum theory of motion. The quantum force creates an initial distribution of kinetic energies that lifts certain trajectories over the transmission threshold while shifting others below this threshold. The view that the quantum force acts when the particle has reached the obstacle is therefore mistaken. Its dominance at early times of the process and disappearance at later times may be a used to improve the efficiency of numerical simulation. The quantum force may be taken into account during the initial period of the motion and 'switched off' once it has become small enough to be inconsequential for the further development of the studied system.

The reflection and transmission coefficients are given by the respective fractions of reflected and transmitted particles. Figure 13.2 shows the obtained transmission probability as a function of the energy E, comparing the quantum trajectory method (QTM) results with those generated by numerical integration of the TDSE.

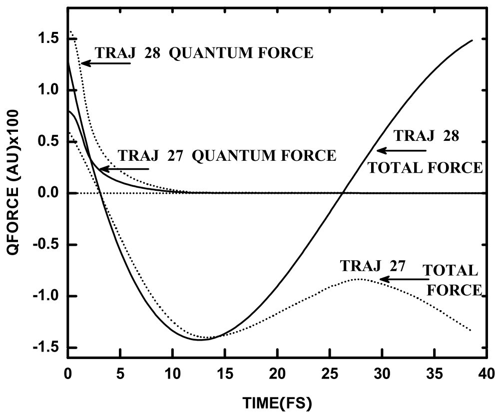

Figure 1: Quantum and total force as a function of time for two characteristic trajectories adjacent to the transmission threshold with initial translational energy $E_0 = (3/4)V_0$. The particles that are more strongly boosted by the quantum force during the first femtoseconds of the motion are transmitted, the remaining ones reflected.(Reprinted with permission from [9]. Copyright (1999) by the American Physical Society.)

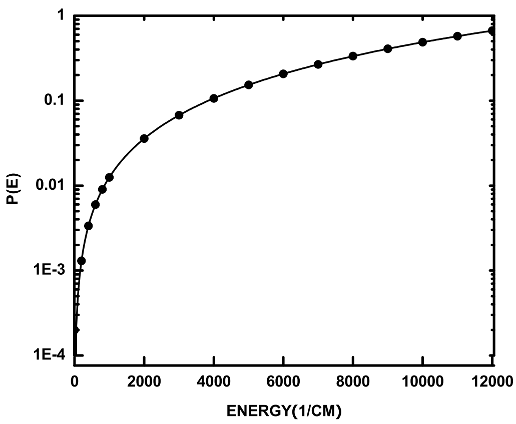

Figure 2: Comparison of the probability for transmission by an Eckart barrier obtained from the quantum trajectory method (black dots) and by solving the TDSE (solid line). (Reprinted with permission from [9]. Copyright (1999) by the American Physical Society.)

The simulation based on the Bohm-de Broglie theory is in excellent agreement with the exact quantum mechanical result over almost four orders of magnitude of the translational energy.

For a long period, the Bohm-de Broglie theory was viewed chiefly as an alternative interpretation of quantum physics that reintroduced 'objectively existing' entities and thus was in opposition to the positivist attitude of the Copenhagen Interpretation, according to which quantum indeterminacy arises as an unavoidable consequence of applying classical categories, such as position and momentum, to the quantum world. With the work of Philippides et al. [5] and later that of R.E.Wyatt and his group [19], however, it became clear that the quantum theory of motion also provides a useful tool for the numerical simulation of quantum processes. In particular, its classical flavor, as manifested by the use of particle trajectories, is very attractive for the treatment of quantum dynamical problems that are too demanding to be addressed by pure wave function propagation methods. At this juncture, we will outline a computational strategy for the application of the Bohm-de Broglie theory to quantum dynamics.

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