Tunnelling Times in Quantum Mechanics

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1 Time in Quantum Mechanics

1.1 Time in Classical Mechanics

In the Hamiltonian formulation of classical mechanics, a system with n degrees of freedom possesses $2n$ independent first-order differential equations in terms of $2n$ independent variables. These variables are the coordinates of the *phase space* of the system, and the $2n$ equations of motion describe the evolution of system in the phase space. n of the independent variables are conventionally chosen to be the generalised coordinates q_i and the other n set to be the conjugate momenta p_i, which obey the Poisson bracket relations: [1]

$$\{q_i, p_j\} = \delta_{ij} \quad \{q_i, q_j\} = \{p_i, p_j\} = 0, \quad i, j = \{1, \dots, n\} \tag{1}$$

The time evolution of the canonical variables is governed by the Hamiltonian $H = H(q_i, p_i)$:

$$\frac{dq_i}{dt} = \{q_i, H\} \quad \frac{dp_i}{dt} = \{p_i, H\} \tag{2}$$

For an infinitesimal variation in time, $\delta t = \delta\tau$, the associated variation in the dynamical variables is:

$$\delta q_i = \{q_i, H\}\delta\tau \quad \delta p_i = \{p_i, H\}\delta\tau \tag{3}$$

q_i and p_i are generalised variables; they are not necessarily positions and momenta, but in the case of a dynamical system comprised of a collection of point particles, the canonical variables are usually the particles' positions ($\boldsymbol{q_i}$) and momenta ($\boldsymbol{p_i}$).

In classical mechanics, physical systems are embedded in a 4-dimensional continuous space-time background, the points of which are assigned coordinates $(t, x, y, z) = (t, \boldsymbol{x})$. It is essential that the *definitions* of these two spaces and their associated coordinates are not conflated. In particular we must distinguish the position variable $\boldsymbol{q}$ from the space-time coordinate $\boldsymbol{x}$. The former defines a point in the phase space of the system (when accompanied by its associated momentum $\boldsymbol{p}$) and is a property of a point particle, whereas the latter is the coordinate of a fixed point in the space-time background in which the dynamical system is embedded. Note we can still introduce both sets of quantities in to equations and relate them, as equations (2) and (3) show.

Immediately this raises the question of whether there exists physical systems that possess a dynamical variable that *resembles* the time coordinate of space-time. Such systems are called *clocks*, more precisely defined as physical systems with a dynamical 'clock' or 'time' variable that behaves similarly to the space-time time coordinate t under time translations. For example, under time translation in which the space-time coordinates transform as:

$$\boldsymbol{x} \to \boldsymbol{x} \quad t \to t + \tau \tag{4}$$

a *linear* clock variable θ and its conjugate momentum η transform as:

$$\eta \to \eta \quad \theta \to \theta + \tau \tag{5}$$

Comparing with (3) we see in the infinitesimal case of (5):

$$\delta\eta = \{\eta, H\}\delta\tau \quad \delta\theta = \{\theta, H\}\delta\tau \tag{6}$$

which implies

$$\{\eta, H\} = 0 \quad \{\theta, H\} = 1 \tag{7}$$

The equation of motion given by (2), $\frac{d\theta}{dt} = 1$ has solution $\theta = t + t_0$.

1.2 Time in Quantum Mechanics

3 definitions for time in QM? In quantum mechanics the state of a particle is encoded in a vector $|\psi\rangle$ in Hilbert space $\mathcal{H}$. Introducing a 1-dimensional continuum position basis to $\mathcal{H}, \{|q\rangle\}, q \in \mathbb{R}$, the state vector $|\psi\rangle$ can be expanded as the integral:

$$|\psi\rangle = \int_{\mathbb{R}} dq \psi(q) \, |q\rangle \tag{8}$$

where $\psi(q)$ is the wave function of the particle. More generally, to describe a system in 3 dimensions requires a wave function $\psi(q_x, q_y, q_z)$. It is important to note that the domain of the wave function is the *configuration space* of the system, $\mathbb{R}^3$, whose coordinates are the generalised coordinates q_i of the system. It is common in elementary quantum mechanics literature for elements of the domain of the wave function to be expressed as (x, y, z), i.e. $\psi = \psi(x, y, z)$. This is clearly in notational conflict with the denotation of coordinates of points of the background space-time in which the quantum system resides.

Measurable quantities or 'observables' are represented by operators on $\mathcal{H}$:

$$\mathcal{O} : \mathcal{H} \to \mathcal{H} \tag{9}$$

Such operators arise through a procedure called canonical quantisation, which prescribes that *dynamical variables* of the Hamiltonian formalism are promoted to operators on $\mathcal{H}$ and their Poisson bracket relations replaced by commutation relations according to:

$$\{,\} \to \frac{1}{i\hbar}[,] \tag{10}$$

One notable omission in this process is the promotion of the time coordinate t to an operator. Given the emphasis placed on distinguishing between space-time coordinates and dynamical variables, the reason is clear: time t is a *space-time coordinate*, and canonical quantisation prescribes that *dynamical variables* are promoted to operators. However this raises the question of whether a time operator exists in quantum mechanics. Resolution to this problem has been historically hindered by a 'proof' offered by Wolfgang Pauli showing that the introduction of a time operator in quantum mechanics is forbidden. It proceeds roughly along the following lines:

Add Pauli proof c.f. Butterfield On Time in Quantum Physics

Observing that this issue arose from attempts to erroneously quantise the *space-time* coordinate t, the problem becomes void and progress can be made by considering the quantisation of timelike *dynamical variables* of physical systems, namely clocks in analogue with the case in classical mechanics mentioned above.

2 Constructing a Quantum Clock

In this section I present a theoretical model of a continuous cyclic quantum clock. The angular variable ϕ plays the role of the clock variable and is represented by the operator $\hat{\Phi}$. An angular momentum operator $\hat{L}$ is also introduced and the two operators in the angular representation are given by:

$$\hat{\Phi} = \phi \quad \hat{L} = -i\frac{d}{d\phi} \tag{11}$$

as is familiar from the theory of angular momentum in quantum mechanics. These operators act on a Hilbert space of square integrable functions of ϕ with domain $[0, 2\pi]$ as:

$$\hat{\Phi} f(\phi) = \phi f(\phi) \quad \hat{L} f(\phi) = -i \frac{d}{d\phi} f(\phi) \tag{12}$$

These operators have eigenvalue equations

$$\hat{\Phi} |\phi\rangle = \phi |\phi\rangle, \phi \in [0, 2\pi] \hat{L} |m\rangle = m |m\rangle, m = 0, \pm 1, \pm 2, \ldots \tag{13}$$

in which the eigenvectors form complete orthonormal sets such that:

$$\langle \phi | \phi' \rangle = \delta(\phi - \phi') \quad \langle m | m' \rangle = \delta_{mm'} \tag{14}$$

Recalling from the theory of angular momentum in quantum mechanics that the $\hat{L}_z = -i \frac{d}{d\phi}$ operator has eigenfunctions $\propto e^{im\phi}$, $|m\rangle$ has wave function $\langle \phi | m \rangle = A e^{im\phi}$ where A is calculated using the normalisation condition to be $(2\pi)^{-\frac{1}{2}}$.
As $\{|m\rangle\}$ form a complex set, $|\phi\rangle$ can be expressed as:

$$|\phi\rangle = (2\pi)^{-\frac{1}{2}} \sum_{-\infty}^{\infty} e^{-im\phi} |m\rangle \tag{15}$$

Introducing the Hamiltonian $\hat{H} = \omega \hat{L}$, the time evolution operator $U(t) = e^{-iHt}$ acts as:

$$\begin{aligned}
\hat{L} e^{-im\phi} |m\rangle &= e^{-im\phi} \hat{L} |m\rangle \text{ by linearity of } \hat{L} i && (16)\\
&= m e^{-im\phi} |m\rangle && (17)\\
\implies e^{iHt} |\phi\rangle &= \sum_{n=0}^{\infty} \frac{(-i\omega t)^n}{n!} \hat{L}^n (2\pi)^{-\frac{1}{2}} \sum_{m=-\infty}^{\infty} e^{-im\phi} |m\rangle && (18)\\
&= (2\pi)^{-\frac{1}{2}} \sum_{n=0}^{\infty} \sum_{m=-\infty}^{\infty} \frac{(-i\omega m t)^n}{n!} e^{-im\phi} |m\rangle && (19)\\
&= (2\pi)^{-\frac{1}{2}} \sum_{m=-\infty}^{\infty} e^{-i\omega m t} e^{-im\phi} |m\rangle && (20)\\
&= |\phi + \omega t\rangle && (21)
\end{aligned}$$

by setting $\omega = 1, \phi$ plays exactly the same role as a time variable t.

We construct a clock with an odd number, $N = 2j + 1$, of states represented by the wavefunctions

$$u_m(\theta) = (2\pi)^{-\frac{1}{2}} e^{im\theta}, m = -j, \ldots, j \text{ and } 0 \leq \theta \leq 2\pi$$

We can construct an alternative orthogonal basis for the clock's wavefunctions

$$v_k(\theta) = N^{-\frac{1}{2}} \sum_{m=-j}^{j} e^{-\frac{2\pi i k m}{N}} u_m \tag{22}$$

$$= (2\pi N)^{-\frac{1}{2}} \sum_{m=-j}^{j} [e^{i(\theta - \frac{2\pi k}{N})}]^m \quad \tilde{m} = m + j \tag{23}$$

$$= (2\pi N)^{-\frac{1}{2}} \sum_{\tilde{m}=0}^{2j} [e^{i(\theta - \frac{2\pi k}{N})}]^{\tilde{m}-j} \tag{24}$$

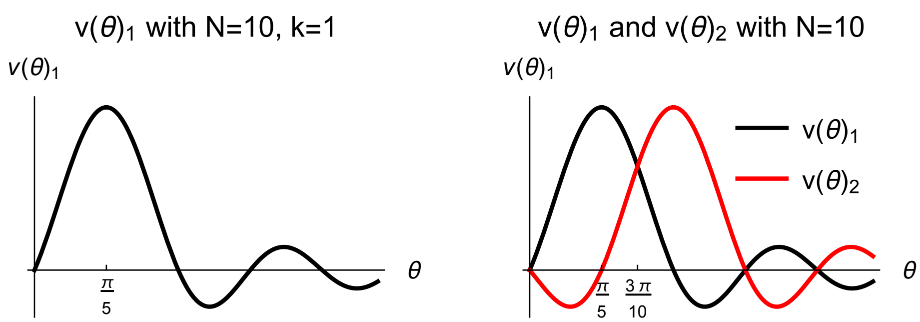
$$= (2\pi N)^{-\frac{1}{2}} [e^{i(\theta - \frac{2\pi k}{N})}]^{\frac{1-N}{2}} \sum_{\tilde{m}=0}^{2j} [e^{i(\theta - \frac{2\pi k}{N})}]^{\tilde{m}} \tag{25}$$

$$= (2\pi N)^{-\frac{1}{2}} [e^{i(\theta - \frac{2\pi k}{N})}]^{\frac{1-N}{2}} \left(\frac{1 - (e^{i(\theta - \frac{2\pi k}{N})})^N}{1 - e^{i(\theta - \frac{2\pi k}{N})}} \right) \tag{26}$$

$$= (2\pi N)^{-\frac{1}{2}} \frac{\sin \frac{N}{2}(\theta - \frac{2\pi k}{N})}{\sin \frac{1}{2}(\theta - \frac{2\pi k}{N})} \tag{27}$$

$$\text{for } k = 0, \ldots, N-1. \tag{28}$$

For large N these functions have a sharp peak at $\theta = \frac{2\pi k}{N}$ which we visualise as pointing to the k^{th} hour with angle uncertainty $\pm\frac{\pi}{N}$:



We can then define projection operators $P_k v_m = \delta_{km} v_m$ and a clock time operator $T_c = \tau \sum k P_k$ where τ is the resolution of the clock. The eigenvectors of T_c are v_k with eigenvalues $t_k = k\tau, k = 0, \ldots, N-1$. Hence measuring T_c yields discrete approximations to the true time, just as analog and digital clocks do.

The clock's Hamiltonian is $H_c = \omega J$ where $\omega = \frac{2\pi}{N\tau}$ and $J = -i\hbar\frac{\partial}{\partial\theta}$

The wavefunctions u_m are eigenfunctions of the Hamiltonian:

$$H_c u_m = m\hbar\omega u_m$$

whence expanding the time evolution operator as a Taylor series gives:

$$e^{-\frac{iH_c t}{\hbar}} u_m = e^{-im\omega t} u_m = (2\pi)^{-\frac{1}{2}} e^{im(\theta - \omega t)} \tag{29}$$

$$\text{and hence} \tag{30}$$

$$\implies e^{-\frac{iH_c \tau}{\hbar}} v_k = N^{-\frac{1}{2}} \sum_m e^{-\frac{2\pi i k m}{N}} e^{-\frac{2\pi i m}{N}} u_m \tag{31}$$

$$= N^{-\frac{1}{2}} \sum_m e^{-2\pi i \frac{m}{N}(k+1)} u_m \tag{32}$$

$$= v_{k+1} \tag{33}$$

3 Larmor Precession

We consider the case of scattering in one dimension with particles of mass m, spin $\frac{1}{2}$ and kinetic energy $E = \frac{\hbar^2 k^2}{2m}$. The particles move along the y-axis with spins polarised with the x-axis and interact with a rectangular barrier,

$$V = \begin{cases} V_0 & -\frac{d}{2} < y < \frac{d}{2} \\ 0 & \text{otherwise} \end{cases} \tag{34}$$

A small magnetic field $\vec{B_0}$ points along the z-axis and is confined to the barrier. As particles enter the barrier, the magnetic field induces a Larmor precession with frequency $\omega_L = \frac{g\mu B_0}{\hbar}$, where g is the gyromagnetic ratio, μ is the absolute value of the magnetic moment. The polarisations of the transmitted and reflected particles are compared with the polarisation of the incident particles.

Particles initially polarised in the x direction obtain a y and z components when tunnelling through the barrier. We know from the Stern-Gerlach experiment that particles polarised int eh x direction can be represented as combinations of particles with z polarisations, $|x;\pm\rangle = \frac{1}{\sqrt{2}}|z;+\rangle \pm \frac{1}{\sqrt{2}}|z;-\rangle$. Outside the barrier, particles have kinetic energy E, independent of their spin. Inside the barrier, the kinetic energy differs by the Zeeman contribution $\pm\frac{\hbar\omega_L}{2}$. The wavefunction inside the barrier will contain an exponentially decaying term $Exp(\kappa_\pm)$, where $\kappa_\pm = (k_0^2 - k^2 \pm \frac{m\omega_L}{\hbar})^{\frac{1}{2}}$, where $\kappa = (k_0^2 - k^2)^{\frac{1}{2}}$ and the sign indicates spin parallel or antiparallel to the field.

We can approximate this in the small ω_L limit as

$$\begin{aligned} \kappa_\pm &= \left(k_0^2 - k^2 \mp \frac{m\omega_L}{\hbar}\right)^{\frac{1}{2}} \\ &= \kappa\left(1 \mp \frac{m\omega_L}{\hbar\kappa^2}\right)^{\frac{1}{2}} \\ &\approx \kappa\left(1 \mp \frac{m\omega_L}{2\hbar\kappa^2}\right) \\ &= \kappa \mp \frac{m\omega_L}{2\hbar\kappa} \end{aligned}$$

Here we examine tunnelling through a barrier in a magnetic field. In this case our Hamiltonian is

$$H = \begin{cases} \left(\frac{p^2}{2m} + V_0\right)\mathbb{1} - \left(\frac{\hbar\omega_L}{2}\right)\sigma_z & |y| \le \frac{d}{2} \\ \left(\frac{p^2}{2m}\right)\mathbb{1} & |y| \ge \frac{d}{2} \end{cases} \tag{35}$$

where $\mathbb{1}$ is the 2×2 identity matrix and $\sigma_x, \sigma_y, \sigma_z$ are the Pauli spin matrices.

H acts on spinors

$$\psi = \begin{pmatrix} \psi_+(y) \\ \psi_-(y) \end{pmatrix} \tag{36}$$

As usual $|\psi_\pm(y)|^2 dy$ is the probability of finding a particle *upon measurement* with spin $\pm\frac{\hbar}{2}$ in the interval $y, y+dy$. We emphasise the 'upon measurement' here as this is an important point of distinction between the orthodox and pilot-wave interpretations addressed in this essay. The incident beam is polarised in the x direction,

$$\psi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{iky} \tag{37}$$

i.e. ψ is an eigenvector of S_x

H is diagonal in the spinor basis so we can solve the scattering problem for particles with spin $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ separately. Our wavefunction is of the form

$$\psi = \begin{cases} A_\pm e^{iky} + B_\pm e^{-iky} & y \le -\frac{d}{2} \\ C_\pm e^{\kappa_\pm y} + D_\pm e^{-\kappa_\pm y} & -\frac{d}{2} \le y \le \frac{d}{2} \\ F_\pm e^{iky} & y \ge \frac{d}{2} \end{cases} \tag{38}$$

We will soon set $A_{\pm} = 1$, corresponding to 1 particle per ??, but maintain it for now to aid a future calculation. Note there is no e^{-iky} term on the right of the barrier, as no particles are reflected.

The effect of the magnetic field B_0 is simply to adjust the height of the barrier, $V_0^{'} = V_0 \pm \frac{\hbar\omega_L}{2}$. Hence we can solve the scattering problem initially assuming no magnetic field, and then adjusting our solution by replacing κ in the field-free problem with $\kappa_{\pm}$. Our job now is to calculate the wavefunction coefficients A, B, C, D, F using the continuity of the wavefunction and its first derivative at the boundaries. This is a lengthy calculation but the results are used so frequently that it is necessary to include a derivation. The results are stated here and derived below:

$$
\begin{aligned}
F &= T^{\frac{1}{2}} e^{i\Delta\phi} e^{-ikd} & \qquad B &= R^{\frac{1}{2}} e^{-\frac{i\pi}{2}} e^{i\Delta\phi} e^{-ikd} \\
C &= \frac{\kappa + ik}{2\kappa} e^{\frac{ikd}{2}} e^{\frac{-\kappa d}{2}} F & \qquad D &= \frac{\kappa - ik}{2\kappa} e^{\frac{ikd}{2}} e^{\frac{\kappa d}{2}} F
\end{aligned} \tag{39}
$$

where T is t:he transmission probability and $R = 1 - T$ is the reflection probability.

First we introduce a new coordinate system so that the boundaries of our barrier become 0, d. Then, denoting our wavefunctions before, inside and after the barrier as ψ_1, ψ_2, ψ_3 respectively, we have:

$$\psi_1 = Ae^{iky} + Be^{-iky} \qquad \psi_1^{'} = Aike^{iky} - ikBe^{-iky} \tag{40}$$

$$\psi_2 = Ce^{-\kappa y} + De^{\kappa y} \qquad \psi_2^{'} = -\kappa Ce^{-\kappa y} + \kappa De^{\kappa y} \tag{41}$$

$$\psi_3 = Fe^{iky} \qquad \psi_3^{'} = ikFe^{iky} \tag{42}$$

Imposing continuity of the wavefunction and its first derivative at the barrier boundaries:

$$\psi_1(0) = \psi_2(0) \implies A + B = C + D \tag{43}$$

$$\psi_1^{'}(0) = \psi_2^{'}(0) \implies ikA - ikB = -\kappa C + \kappa D \tag{44}$$

$$\psi_2(d) = \psi_3(d) \implies Ce^{-\kappa d} + De^{\kappa d} = Fe^{ikd} \tag{45}$$

$$\psi_2^{'}(d) = \psi_3^{'}(d) \implies -\kappa Ce^{-\kappa d} + \kappa De^{\kappa d} = ikFe^{ikd} \tag{46}$$

$$ik(43) + (44) \implies 2ikA = C(ik - \kappa) + D(ik + \kappa) \tag{47}$$

$$ik(43) - (44) \implies 2ikB = C(ik + \kappa) + D(ik - \kappa) \tag{48}$$

$$\kappa(45) - (46) \implies 2\kappa Ce^{\kappa d} = Fe^{ikd}(\kappa - ik) \tag{49}$$

$$\kappa(45) + (46) \implies 2\kappa De^{\kappa d} = Fe^{ikd}(\kappa + ik) \tag{50}$$

Inserting equations (49) and (50) into equation (47) we arrive at:

$$2ikA = -\frac{(ik - \kappa)^2}{2\kappa} Fe^{(ik+\kappa)d} + \frac{(ik + \kappa)^2}{2p} Fe^{(ik-\kappa)d} \tag{51}$$

$$\implies 4\kappa ikAe^{-ikd} = F[(k^2 - \kappa^2)(e^{\kappa d} - e^{-\kappa d}) + 2ik\kappa(e^{\kappa d} + e^{-\kappa d})] \tag{52}$$

$$= F[2(k^2 - \kappa^2)\sinh \kappa d + 4ik\kappa \cosh \kappa d] \tag{53}$$

We hence arrive at our first result, the transmission probability $T = \frac{|F|^2}{|A|^2}$:

$$T = [1 + \frac{(k^2 + \kappa^2)^2 \sinh^2 \kappa d}{4k^2\kappa^2}]^{-1}.$$

and, by writing F in polar form $F = |F|e^{i\theta}$, the phase change across the barrier: i

$$F \propto 4k^2\kappa^2 \cosh\kappa d e^{-ikd} + i2k\kappa(k^2-\kappa^2)\sinh\kappa d e^{-ikd} \tag{54}$$

$$\implies \Delta\phi := arg(F) = \arctan\left(\frac{\mathrm{Im}(F)}{\mathrm{Re}(F)}\right) = \arctan\left(\frac{(k^2-\kappa^2)}{2k\kappa}\tanh\kappa d\right) \tag{55}$$

$$\implies Fe^{ikx}|_{x=d} - e^{ikx}|_{x=0} = |F|e^{i\Delta\phi}e^{ik(d-d)} - 1 \tag{56}$$

and so the phase change $= \Delta\phi$ (57)

It is clear now why we left the coefficient A explicit, but from now on it will be set to A = 1. Rearranging (53) for F, we can compare with the final result in (39) and factorise out $T^{\frac{1}{2}}$:

$$F = T^{\frac{1}{2}}e^{-ikd} \times \frac{(k^2-\kappa^2)i\sinh\kappa d + 2k\kappa\cosh(\kappa d)}{\sqrt{(k^2+\kappa^2)^2\sinh^2\kappa d + 4k^2\kappa^2}}$$

This yields the identification

$$e^{i\Delta\phi} = \frac{(k^2-\kappa^2)i\sinh\kappa d + 2k\kappa\cosh\kappa d}{\sqrt{(k^2+\kappa^2)\sinh^2(\kappa d) + 4k^2\kappa^2}} \tag{58}$$

$$= \frac{(k^2-\kappa^2)i\tanh\kappa d + 2k\kappa}{\sqrt{(k^2-\kappa^2)^2\tanh^2\kappa d + 4k^2\kappa^2}} \tag{59}$$

Expanding the left hand side into real and imaginary parts and comparing coefficients we deduce:

$$\tan\Delta\phi = \frac{(k^2-\kappa^2)\tanh(\kappa d)}{2k\kappa}$$

The result for B follows along similar lines and results for C and D follow immediately from equations (49) and (50). We note that our final results are independent of the coordinate system used (up to scaling by a multiplicative constant) so the result also holds in our other coordinate system.

References

[1] Goldstein