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Quantum Mechanics via Path Amplitudes

JAYANT V. NARLIKAR
Inter-University Centre for Astronomy and Astrophysics
Ganeshkhind, Pune 411007

1. Introduction

One of the culture shocks encountered by a physics student occurs when first faced with quantum mechanics. The smug feeling that the clear and deterministic Newtonian mechanics can in principle explain all observed phenomena, is shattered with the realization that it fails to work at the microscopic level of an atom. A further jolt is given when new concepts ate introduced, such as: (a) particle-wave duality, (b) the uncertainty principle, (c) the operator nature of dynamical variables, (d) the introduction of a complex number for the probability amplitude to understand a real experiment.

This culture shock is understandable in the context of the history of the early growth of the subject when top scientists were also confounded by the way nature works at the microscopic level. From the empirical approach of Bohr to the mathematical formulation by Dirac, through the ideas contributed by De Broglie, Schrödinger and Heisenberg, there were several discussions of epistemological nature among leading scientists, including the celebrated one between Bohr and Einstein. Even today, the foundational aspects of quantum mechanics are subject to discussions around coffee tables and specialist conferences.

Nevertheless the student encountering the subject for the first time can be spared some of the conceptual problems through which the pioneers had to go. Having encountered the same problems myself as a student, I would like to share my experience with the reader.

To put it in a nutshell, the major conceptual issue is of continuity: of knowing when classical mechanics begins to fail and the regime of quantum mechanics takes over, and how the transition takes place in the meaning of the dynamical variables. It is here that I found the usual operator approach to quantum mechanics inadequate. The path integral approach introduced by Feynman is far more appealing to intuition. This article will highlight the introductory aspects of this approach.

2. Action, Paths and Probability Amplitude

Let us begin by recalling the general approach to classical Newtonian mechanics.

Take the simple case of a particle of mass m moving in one dimension (denoted by the x-coordinate) under a potential $V(x)$. The particle is to start from position x_1 at time t_1, and is to arrive at position x_2 at time t_2. How will it go? In short, we need to determine the path Γ_c, between these two points in the $x - t$ plane, followed by the particle. We will label these points P_1 and P_2 respectively.

The classical method is to define an action for the problem by:

$$S = \int_{\Gamma} L\,[x, \dot{x}, t]\, dt \ , \tag{1}$$

where the Lagrangain L is given in this case by

$$L = \frac{1}{2} m\, \dot{x}^2 - V(x) \ . \tag{2}$$

The path Γ along which the action is evaluated is specified by a function $x = x(t)$.

The next step involves determining the path Γ along which the action is stationary. That is, for small variations of the path function $x(t) \rightarrow x(t) + \delta x(t)$, the change in the action, δS, should vanish. The requirement is that paths are allowed to be varied provided their endpoints are fixed. In the above case this procedure leads to the familiar Newtonian equation of motion:

$$m\, \ddot{x} = -V'(x) \ . \tag{3}$$

The deterministic nature of classical mechanics is seen from the fact that once we solve the above differential equation with the two end-point conditions $x(t_1) = x_1, x(t_2) = x_2$, the function $x(t)$ gets completely fixed. This is the classical path Γ_c.

Now even in classical physics this procedure is mysterious! Why write an action and why stationarize it? Why do we get the relevant equation of motion by this method?

This is where the intuitive character of the path integral approach makes its vital contribution. We will return to these questions after discussing this approach to quantum mechanics.

The double slit experiment discussed in most introductory tests on quantum mechanics tells us that the path of a microscopic particle like an electron cannot be specified with absolute certainty. In other words, in the above problem, we may have to allow for the possibility that the electron travelled from P_1 to P_2 by some other path than Γ_c. In fact any geometrically possible path that does not reverse back in time is permissible. (We are considering here the case of non-relativistic motion and so the restriction of the speed of light as the upper limit on $|\dot{x}|$ does not apply.) Figure 1 illustrates the scenario.

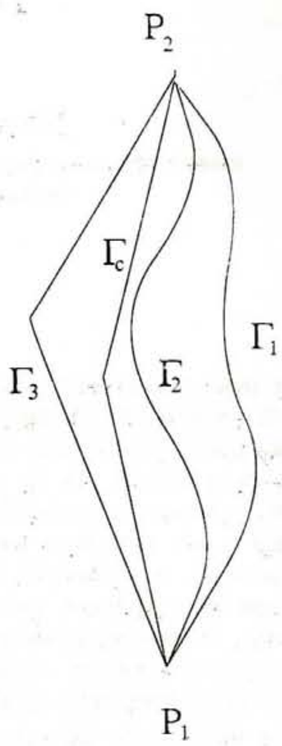

Figure 1 Typical paths Γ_1, Γ_2, Γ_3, . . . connecting P_1 to P_2. the classical path Γ_c is the one along which $\delta S = 0$.

How do we allow for this multi-path possibility? Fenyman gave a simple prescription to settle this question. for each path Γ, given by a function $x(t)$ connecting the end points, calculate the action functional $S[x(t)]$. Then the probability amplitude for a particle to go from P_1 to P_2 along this path is given by

$$P[\Gamma] = \text{constant.exp}\left[\frac{iS\,[x\,(t)]}{\hbar}\right] \tag{4}$$

To fix ideas, let us denote the constant on the right hand side by A^{-1}. It will in general be a complex number. The particle may be go from P_1 to P_2 along one of the possible paths, but we cannot tell which. The probability for each path is the same, being the square of the modulus of the probability amplitude. However, the phase of each amplitude is different, being path dependent. Thus when we ask for the *total* probability amplitude the various path amplitudes will interfere. Therein lies the crux of the difference between classical and quantum mechanics.

First note that we have introduced the Planck constant through the term $\hbar$. So far its role has only been to provide a dimensional constant to make the exponent in the above equation dimensionless (— a necessary requirement if we are to take an exponential). This constant could be anything with the dimensions of action, that is, with mass-length-time combination of ML^2T^{-1}.

So when we add the probability amplitudes, we are basically adding complex numbers lying on the unit circle, and then multiplying the result by the constant term A^{-1}. Now recall that for macroscopic motions the action functional S is large compared to $\hbar$. Take for example, a particle of mass 20 kg moving at the speed of 10 meters per second for 10 seconds under no forces, then the action for this motion is $S \sim 0.5 \times 20 \times 10^2 \times 10 = 10^4$ in MKS units. When divided by $\hbar$ we get $S/\hbar \sim 10^{38}$, i.e. an enormously large number. Thus even for relatively close-by paths, the contributions to the phase of the complex number will be wildly different. So when we add different contributions from the various paths, the net effect of randomly distributed points on the unit circle is zero.

Except, that is one special case. Suppose that there is a group of neighbouring paths for which the action happens to be the same. For such paths, the phases add coherently and there is a net non-zero contribution to the probability amplitude. But such paths are none other than those close to the classical path Γ_c for which $\delta S = 0$.

Thus the prescription of adding probability amplitudes tells us that in the classical limit when $S \gg \hbar$, the dynamical system will choose the spacetime path along which the action is stationary.

We thus arrive at a rationale for the principle of stationary action for classical mechanics.

3 Application to Quantum Mechanics

Let us take another example at the other end, when the classical action is expected to be comparable to $\hbar$. We take the familiar example of the hydrogen atom. Let m stand for the mass of the electron, e for the magnitude of its charge, and $\mathbf{r}$ for its distance vector relative to the nucleus. The action for the motion of the electron is then given by

$$S = \int \left[\frac{1}{2} m \dot{\mathbf{r}}^2 + \frac{e^2}{r} \right] dt \ . \qquad (5)$$

Let us calculate the action on the assumption that the electron goes round the nucleus with period T. Then, for radius of the orbit equal to a, we get from Newton's laws of motion

$$T = 2 \pi m^{1/2} a^{3/2} e^{-1} \qquad (6)$$

Taking the time interval of the integral to be T, the order of magnitude of the action is then

$$S \sim (e^2/2a) \times T \sim \pi m^{1/2} a^{1/2} e. \qquad (7)$$

Now if we insist on using classical dynamics for this system, we must have $S \gg \hbar$. From the above relation,

$$a \gg \frac{\hbar^2}{m e^2} \ . \qquad (8)$$

In reality, the right hand side of the above equation is comparable to the size of the hydrogen atom!

What this analysis tells us is that classical dynamics cannot be applied to the study of the H-atom. Or, to put argument the other way round, if we apply the criterion $S \sim \hbar$ to the hydrogen atom we are able to deduce its size.

So the conclusion is that for quantum mechanical systems the action is comparable to the Planck constant.

4. De Broglie Wavelength and Frequency

Let us next consider the semiclassical situation where the total path amplitude can be approximated by summing over the amplitudes over paths in the neighbourhood of the classical path Γ_c. We may then write the amplitude to go from P_1 to P_2 as

$$K\,[P_2; P_1] \sim \exp\left[\frac{i\,S_c}{\hbar}\right] , \qquad (9)$$

where the action S_c has been evaluated along the classical 'stationary action' path Γ_c. Consider now the behaviour of this function at the end-point P_2. In the situation where the action is large compared to $\hbar$, a small variation of space coordinate x_2 will cause a rapid variation of K. The change in phase of K per unit displacement of x_2 will be given by

$$k = \frac{1}{\hbar} \cdot \frac{\partial\, S_c\,(x_2)}{\partial\, x_2} . \qquad (10)$$

However, classical mechanics tells us that the classical momentum of the particle when it arrives at P_2 is

$$p_2 = \left[\frac{\partial\, S_c}{\partial\, x}\right]_{P_2} \qquad (11)$$

Thus, we recover the quantum mechanical interpretation that the particle has a wavenumber given by

$$k = p/\hbar , \qquad (12)$$

that is, its momentum is related to its 'wavelength' by the De Broglie relation $\lambda = h/p$.

A similar interpretation can be given to the 'frequency' of the probability amplitude in terms of energy of the particle as interpreted classically.

5. Concluding Remarks

This is just an elementary glimpse into an off-the-beaten-track approach to quantum mechanics. To get into further quantitative details, one needs to evolve a method of 'summing over all paths', a notion that takes us to the study of path integrals. I can do no better than refer the reader to the classic book by Feynman and Hibbs[1] or to the original paper by Feynman.[2] There one can see how to arrive at the various 'operators' that smoothly merge with the definitions of their classical counterparts.

References

1. R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, Inc., New York (1965).
2. R.P. Feynman, "Space-Time Approach to Non-Relativistic Quantum Mechanics", *Rev. Mod. Phys.*, 20, 367 (1948).