Snippets of Physics

13. The Optics of Particles

T Padmanabhan

T Padmanabhan works at IUCAA, Pune and is interested in all areas of theoretical physics, especially those which have something to do with gravity.

The probability amplitude for a particle to propagate from event to event in spacetime shows some nice similarities with the corresponding propagator for the electromagnetic wave amplitude discussed in the last installment. In fact, this analogy provides an interesting insight into the transition from quantum field theory to quantum mechanics!

In classical mechanics, the motion of a particle with position $\mathbf{x}(t)$ under the action of a (time independent) potential $V(\mathbf{x})$ is determined through the Newton's law of motion $m\ddot{\mathbf{x}} = -\nabla V$. Given the initial position $\mathbf{x}(0)$ and velocity $\mathbf{v}(0)$ at $t = 0$ we can integrate this equation to determine the trajectory. All other physical observables in classical mechanics can be obtained from the trajectory $\mathbf{x}(t)$.

What is the corresponding situation in quantum mechanics? Here the wavefunction of the particle $\psi(t, \mathbf{x})$ contains complete information about the state of the system and satisfies the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \equiv H\psi. \quad (1)$$

Given the wavefunction $\psi(0, \mathbf{x})$ at $t = 0$ we can integrate this equation and obtain the wavefunction at any later time. But, unlike in the case of classical mechanics, there is a nice way of separating the dynamical evolution from the initial condition in the case of quantum mechanics which we shall first describe. To keep the discussion somewhat general we will assume that the

Keywords
Optics, waves.

space has D dimensions with the usual choices being $D = 1, 2, 3$.

We know that when the potential is independent of time, equation (1) has energy eigenstates which satisfy the eigenvalue equation $H\phi_n(\mathbf{x}) = E_n\phi_n(\mathbf{x})$. Using these eigenfunctions we can expand the initial wavefunction $\psi(0, \mathbf{x})$ in terms of the energy eigenfunctions as

$$\psi(0, \mathbf{x}) = \sum_n c_n\phi_n(\mathbf{x}); \quad c_n = \int \mathrm{d}\mathbf{y}\, \psi(0, \mathbf{y})\phi_n^*(\mathbf{y}), \quad (2)$$

where the expression for c_n follows from the orthonormality of the energy eigenfunctions and the spatial integrations are over the D-dimensional space. Since the energy eigenfunction evolves in time with a phase factor $\exp(-iE_nt/\hbar)$, it follows that the wavefunction at time t is given by

$$\psi(t, \mathbf{x}) = \sum_n c_n\phi_n(\mathbf{x})e^{-iE_nt/\hbar}, \quad (3)$$

which, in principle, solves the problem. Actually, we can do better by expressing the c_ns in (3) in terms of $\psi(0, \mathbf{x})$ using the second relation in (2). This gives

$$\begin{aligned} \psi(t, \mathbf{x}) &= \int d\mathbf{y}\, \psi(0, \mathbf{y}) \sum_n \phi_n(\mathbf{x})\phi_n^*(\mathbf{y})e^{-iE_nt/\hbar} \\ &\equiv \int d\mathbf{y}\, K(t, \mathbf{x}; 0, \mathbf{y})\psi(0, \mathbf{y}), \quad (4) \end{aligned}$$

where we have defined the function – usually called the propagator or kernel – by

$$K(t, \mathbf{x}; 0, \mathbf{y}) = \sum_n \phi_n^*(\mathbf{y})\phi_n(\mathbf{x})e^{-iE_nt/\hbar}. \quad (5)$$

It is obvious that the propagator $K(t, \mathbf{x}; 0, \mathbf{y})$ carries complete information about the dynamical evolution of the system and can be computed once the Hamiltonian

It is obvious that the propagator $K(t,\mathbf{x};0,\mathbf{y})$ carries complete information about the dynamical evolution of the system.

Curiously enough, such a separation has no direct analog in the case of classical mechanics.

H is known, in terms of its eigenfunctions and the eigenvalues. What is more, equation (4) nicely separates the dynamics, encoded in $K(t, \mathbf{x}; 0, \mathbf{y})$, from the initial condition encoded in $\psi(0, \mathbf{y})$. Curiously enough, such a separation has no direct analog in the case of classical mechanics.

Since $\psi(0, \mathbf{y})$ gives the amplitude to find the particle around $\mathbf{y}$ at $t = 0$, it follows that $K(t, \mathbf{x}; 0, \mathbf{y})$ can be thought of as the probability amplitude for a quantum particle to propagate from the event $(0, \mathbf{y})$ to the event $(t, \mathbf{x})$. Of course, since the potential is independent of time, we can use time translation invariance to write an expression for $K(t_2, \mathbf{x}_2; t_1, \mathbf{x}_1)$ by replacing $E_n t/\hbar$ in (5) by $(E_n/\hbar)(t_2 - t_1)$. For this interpretation to be valid the propagator must satisfy the integral condition:

$$K(t_3, \mathbf{x}_3; t_1, \mathbf{x}_1) = \int \mathrm{d}\mathbf{x}_2 K(t_3, \mathbf{x}_3; t_2, \mathbf{x}_2) K(t_2, \mathbf{x}_2; t_1, \mathbf{x}_1). \tag{6}$$

Using the definition in (5) and the orthonormality of eigenfunctions, you can prove that this is indeed true. Note that this is a nontrivial condition: At the intermediate event we integrate only over $\mathbf{x}_2$ leaving t_2 alone; nevertheless, the final result – and the left hand side – is independent of t_2. So the propagator actually propagates the particle from event to event.

Note that equation (6) is a nontrivial condition: At the intermediate event we integrate only over $\mathbf{x}_2$ leaving t_2 alone; nevertheless, the final result – and the left hand side – is independent of t_2.

Since ϕ_ns are energy eigenfunctions, it is also straightforward to verify that the propagator satisfies the Schrödinger equation

$$\left(i\hbar \frac{\partial}{\partial t} - H \right) K(t, \mathbf{x}; 0, \mathbf{y}) = 0, \tag{7}$$

with the special initial condition

$$\lim_{t \to 0} K(t, \mathbf{x}; 0, \mathbf{y}) = \delta_D(\mathbf{x} - \mathbf{y}). \tag{8}$$

This condition can also be obtained easily from (4) by taking the limit of $t \to 0$.

After this preamble about the propagator, we will turn to the key topic of this installment. To introduce it, let us work out the propagator for a free particle ($V = 0$) using the expression in (5). In the case of a free particle the energy eigenfunctions and eigenvalues can be taken to be labelled by a wavenumber $\mathbf{p}$ instead of a discrete index n with

$$\phi_{\mathbf{p}}(\mathbf{x}) = \frac{1}{(2\pi)^{D/2}} \exp i(\mathbf{p}\cdot\mathbf{x}); \qquad E_{\mathbf{p}} = \frac{\hbar^2 p^2}{2m}. \tag{9}$$

The normalization of $\phi_{\mathbf{p}}(\mathbf{x})$ is somewhat arbitrary but we use the convention that momentum space integrals come with a measure $d\mathbf{p}$ so that the orthonormality condition reads as

$$\int \mathrm{d}\mathbf{p}\phi_{\mathbf{p}}(\mathbf{x})\phi^*_{\mathbf{p}}(\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}). \tag{10}$$

The propagator is now given by an expression similar to (5) but with an integral over $\mathbf{p}$ rather than a sum over the discrete index n. Hence we get

$$\begin{aligned} K(t,\mathbf{x};0,\mathbf{y}) &= \int \frac{\mathrm{d}\mathbf{p}}{(2\pi)^D} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})/\hbar} e^{-ip^2\hbar t/2m} \\ &= \left(\frac{m}{2\pi i\hbar t}\right)^{D/2} \exp\left[\frac{im}{\hbar}\frac{(\mathbf{x}-\mathbf{y})^2}{2t}\right], \end{aligned} \tag{11}$$

where D is the dimension of space (1, 2 or 3) in which the particle is moving. (The integral is just the D-dimensional Fourier transform of a Gaussian which separates out in each of the dimensions.) We can verify directly that $K(t,\mathbf{x};0,\mathbf{y})$ satisfies (7) and (8). It is also obvious that it satisfies the "normalization condition"

$$\int \mathrm{d}\mathbf{x}\ K(t,\mathbf{x};0,\mathbf{y}) = 1. \tag{12}$$

Usually in quantum mechanics we normalize the probabilities and not the probability amplitudes. But this is an exception to the rule in which probability amplitude

Equation (12) is an exception to the rule in which probability amplitude for propagation from event to event comes out normalized to unity.

for propagation from event to event comes out normalized to unity.

There is a conventional interpretation of the phase of the propagator in (11) which we will now describe. To do this, let us consider the action for the free particle in classical mechanics given by

$$\mathcal{A}(t, \mathbf{x}; 0, \mathbf{y}) = \frac{m}{2} \int_0^t \mathrm{d}t \, |\dot{\mathbf{x}}|^2, \tag{13}$$

which is defined for any trajectory $\mathbf{x}(t)$ that connects the two end points. In particular, we can determine the classical trajectory $\mathbf{x}_c(t)$ from extremising the action and evaluate the classical value of the action $\mathcal{A}_c(t, \mathbf{x}; 0, \mathbf{y})$ for this particular classical trajectory. For the free particle, this is trivial to evaluate and is given by

$$\mathcal{A}_c(t, \mathbf{x}; 0, \mathbf{y}) = \frac{m}{2} \frac{(\mathbf{x} - \mathbf{y})^2}{t}, \tag{14}$$

so that the propagator in (11) can be expressed in the form

$$K(t, \mathbf{x}; 0, \mathbf{y}) = N(t) \exp\left[\frac{i}{\hbar} \mathcal{A}_c(t, \mathbf{x}; 0, \mathbf{y})\right]. \tag{15}$$

We see that the phase of the propagator can be interpreted as just the classical value of the action divided by $\hbar$.

The situation is actually better than this. Let us consider, instead of the classical path, any arbitrary path connecting the two events (labelled 1 and 2) we are interested in. Since one cannot measure position and velocity of a particle simultaneously in quantum mechanics, it does not make sense to say that the particle went from one point to another along a particular trajectory. The best we can say is that there is some amplitude $\mathcal{P}(2; 1|\mathbf{x}(t)) \equiv \mathcal{P}(t_2, \mathbf{x}_2; t_1, \mathbf{x}_1|\mathbf{x}(t))$ for the particle to choose a particular path $\mathbf{x}(t)$. We now postulate, following Dirac and Feynman, that this amplitude is given by

We see that the phase of the propagator can be interpreted as just the classical value of the action divided by $\hbar$.

$\mathcal{P}(2;1|\mathbf{x}(t)) = \exp(i\mathcal{A}[2;1|\mathbf{x}(t)]/\hbar)$. Then the total amplitude for propagation from event 1 to event 2 (which, of course, is our propagator) must be given by

$$K(2;1) = \sum_{paths} \mathcal{P}(2;1|\mathbf{x}(t)) = \sum_{\mathbf{x}(t)} \exp(i\mathcal{A}[2;1|\mathbf{x}(t)]/\hbar), \quad (16)$$

In general, it is not easy to define and evaluate the sum in (16) but something interesting happens if the action contains no terms which are more than quadratic in velocity or position.

where the summation symbol indicates that we have to sum over all paths $\mathbf{x}(t)$ connecting the two events. In general, it is not easy to define and evaluate this sum but something interesting happens if the action contains no terms which are more than quadratic in velocity or position. In these cases, we begin by writing any arbitrary path – over which we have to sum – in terms of the classical path $\mathbf{x}_c(t)$ plus a deviation from it: that is, we write $\mathbf{x}(t) = \mathbf{x}_c(t) + \mathbf{r}(t)$. Summing over all $\mathbf{x}(t)$ is the same as summing over all $\mathbf{r}(t)$ but the 'boundary conditions' on $\mathbf{r}(t)$ are easier to handle. Since both the classical path $\mathbf{x}_c(t)$ and any arbitrary path $\mathbf{x}(t)$ connect the same end points, the $\mathbf{r}(t)$ must vanish at the end points. Further, if the action has only up to quadratic terms in $\mathbf{x}(t)$, then it splits up as the sum:

$$\begin{aligned} \mathcal{A}[\mathbf{x}(t)] &= \mathcal{A}[\mathbf{x}_c(t) + \mathbf{r}(t)] \\ &= \mathcal{A}[\mathbf{x}_c(t)] + \mathcal{A}_{lin}[\mathbf{x}_c(t), \mathbf{r}(t)] + \mathcal{A}_{quad}[\mathbf{r}(t)], \quad (17) \end{aligned}$$

where $\mathcal{A}_{lin}$ is linear in $\mathbf{x}(t)$ and $\mathbf{r}(t)$ while $\mathcal{A}_{quad}$ is quadratic in $\mathbf{r}(t)$. (This is essentially paraphrasing the formula for $(a+b)^2$!). But recall that the classical path is an extremum of the action; so the change in action when the path changes by a deviation $\mathbf{r}(t)$ has to be to quadratic order in $\mathbf{r}$. Therefore, $\mathcal{A}_{lin} = 0$ and the sum over paths in (16) can be written as:

$$\begin{aligned} K(2;1) &= \sum_{\mathbf{x}(t)} \exp(i\mathcal{A}[2;1|\mathbf{x}(t)]/\hbar) \\ &= \exp(i\mathcal{A}[2;1|\mathbf{x}_c(t)]/\hbar) \sum_{\mathbf{r}(t)} \exp(i\mathcal{A}_{quad}[\mathbf{r}(t)]/\hbar). \quad (18) \end{aligned}$$

The sum over $\mathbf{r}(t)$ in (18) (which we haven't even defined properly!) can only be a function of t_2,t_1. We get the neat result that for all actions which have only up to quadratic terms in their variables, the propagator has the form in (15).

The crucial point is that the sum over $\mathbf{r}(t)$ is done with the condition $\mathbf{r}(t_2) = \mathbf{r}(t_1) = 0$ and hence it does not depend on $\mathbf{x}_1, \mathbf{x}_2$. So the sum over $\mathbf{r}(t)$ in (18) (which we haven't even defined properly!) can only be a function of t_2, t_1. We get the neat result that for all actions which have only up to quadratic terms in their variables, the propagator has the form in (15). (In fact, one can also determine $N(t_2, t_1)$ using the condition (6) but we won't go into that.). For all these cases, of which the free particle is a special case, the phase of the propagator is just the classical action.

This is all nice but in non-relativistic mechanics the action functional in (13) has no simple geometrical interpretation. We will now provide an alternative perspective on the phase of the propagator which will lead to a geometric insight.

The most remarkable feature about the propagator in (11), from this alternative perspective, is that we have already seen this expression in the last installment in connection with the propagation of electromagnetic waves along the z-direction! There we had the expression[1] for a propagator which is reproduced here for your convenience:

$$G\left(z - z'; \mathbf{x}_\perp - \mathbf{x}'_\perp\right) =$$

$$\left(\frac{\omega}{2\pi i c}\right) \frac{1}{|z - z'|} \exp\left[\frac{i\omega}{2c} \frac{\left(\mathbf{x}_\perp - \mathbf{x}'_\perp\right)^2}{(z - z')}\right]. \qquad (19)$$

[1] See equation (7) in *Resonance*, Vol.13, p.1100, December 2008.

Comparing (19) with (11) we see the following correspondence. The $(z - z')/c$, which is the time of light travel along the z-axis (along which the wave is propagating) is analogous to time t in quantum mechanics. The two transverse spatial directions in the case of electromagnetic wave propagation are analogous to the spatial coordinates in quantum mechanics in 2-dimensions; so we can set $D = 2$ in (11). The frequency should get mapped to the relation $\hbar\omega = mc^2$ which is essentially the frequency associated with the Compton wavelength of the particle. This will make the propagators identical! Obviously, this deserves further probing especially since the correspondence brings in a c factor when we thought we are doing nonrelativistic quantum mechanics.

Obviously, this deserves further probing especially since the correspondence brings in a *c* factor when we thought we are doing nonrelativistic quantum mechanics.

In the case of the propagation of electromagnetic wave amplitude, we were propagating it along the positive z-direction with $\mathbf{x}$ and $\mathbf{y}$ acting as two transverse directions. In the case of quantum mechanics, we are propagating the amplitude for a particle along the positive t-direction with all the spatial coordinates acting as 'transverse directions'. In the language of paraxial optics, the special axis is along the time direction in quantum mechanics.

But we know that paraxial optics is just an approximation to a more exact propagation in terms of the wave equation. In the wave equation for the electromagnetic wave, the three coordinates (x, y, z) appear quite symmetrically and to obtain paraxial limit, we choose one axis (z-axis) as special and propagate the amplitude along the positive direction. This is why the propagator in (19) has the x, y coordinates appearing differently compared to the z-axis. Doing a bit of reverse engineering we can ask the question: If the quantum mechanical propagator is some kind of paraxial optics limit of a more exact theory, what will it be?

An obvious way to explore the situation is to restore the symmetry between z and x, y in optics and, similarly, restore the symmetry between t and $\mathbf{x}$ in quantum mechanics. We can do this if we recall the interpretation of the phase as due to the path difference in the case of electromagnetic wave. The relevant equation[2] is again reproduced below:

[2] See equation (9) in *Resonance*, Vol.13, p.1103, December 2008.

$$k\Delta s = \frac{\omega}{c}\left[\sqrt{\left(\mathbf{x}_\perp - \mathbf{x}'_\perp\right)^2 + (z - z')^2} - (z - z')\right]$$

$$\cong \frac{\omega}{c}\left[\frac{1}{2}\frac{(\mathbf{x}_\perp - \mathbf{x}'_\perp)^2}{(z-z')}\right]. \tag{20}$$

We use the fact that a path difference Δs between two points in space will introduce a phase difference of $k\Delta s$ in a propagating wave. The paraxial optics results when the transverse displacements are small compared to the longitudinal distance. Taking a cue from this, let us construct the quantity

$$\frac{l(t,\mathbf{x};0,\mathbf{y}) - ct}{\lambda} \equiv \frac{mc}{\hbar}\left\{\left[c^2t^2 - (\mathbf{x}-\mathbf{y})^2\right]^{1/2} - ct\right\}, \tag{21}$$

where $l(t,\mathbf{x};0,\mathbf{y})$ is the special relativistic spacetime interval between the two events. We are subtracting from it the 'paraxial distance' ct along the time direction and dividing by $\lambda \equiv (\hbar/mc)$ which is the Compton wavelength of the particle. This is exactly the construction suggested by the correspondence between (19) and (11), discussed previously, except for using the special relativistic line interval, with a minus sign between space and time. The paraxial limit now arises as the nonrelativistic limit of this expression in (21) when $c \to \infty$; this is given by

$$\frac{l - ct}{\lambda} \cong -\frac{m}{2}\frac{(\mathbf{x}-\mathbf{y})^2}{\hbar t}, \tag{22}$$

We are subtracting from $l(t, x; 0, y)$ the 'paraxial distance' *ct* along the time direction and dividing by $\lambda \equiv (\hbar / mc)$ which is the Compton wavelength of the particle.

which is precisely the phase of the propagator in (11) except for a sign. So the propagator can be thought of as the nonrelativistic limit of the function

$$K(t,\mathbf{x};0,\mathbf{y}) = N(t)e^{i(mc^2/\hbar)t}\exp\left(-i\left[\frac{l(t,\mathbf{x};0,\mathbf{y})}{\lambda}\right]\right). \tag{23}$$

So the phase of the propagator is just the proper distance between the two events, in units of the Compton wavelength, just as the phase in the case of the electromagnetic wave propagator is the path length in units of the wavelength. (The extra factor $(mc^2/\hbar)t$ does not contribute to the propagation integral in (4) and goes for a ride; we can ignore it but if you want you can also think of it as arising from the energy being shifted by mc^2.). We can think of the path difference between a straight path along the time direction (with $\mathbf{x} = \mathbf{y}$) and another specified path as contributing a phase l/λ to the propagator. This geometric interpretation is lost for the phase in the paraxial limit (in the case of electromagnetic theory) and in the nonrelativistic limit (in the case of a particle).

This geometric interpretation is lost for the phase in the paraxial limit (in the case of electromagnetic theory) and in the nonrelativistic limit (in the case of a particle).

This extension suggests that the phase in the relativistic case can be related to the corresponding action. The action for a free particle in special relativity is given by

$$\mathcal{A}_R(t, \mathbf{x}; 0, \mathbf{y}) = -mc^2 \int_0^t \mathrm{d}t \left(1 - \frac{v^2}{c^2}\right)^{1/2}. \qquad (24)$$

Once again, evaluating this for a relativistic classical trajectory we get

$$\begin{aligned} \mathcal{A}_R^c(t, \mathbf{x}; 0, \mathbf{y}) &= -mc^2 t \left[1 - \frac{(\mathbf{x} - \mathbf{y})^2}{c^2 t^2}\right]^{1/2} \\ &= -mc \left[c^2 t^2 - (\mathbf{x} - \mathbf{y})^2\right]^{1/2}, \qquad (25) \end{aligned}$$

which is essentially the interval between the two events in the spacetime. This suggests expressing the propagator for the relativistic free particle in the form

$$K(t, \mathbf{x}; 0, \mathbf{y}) = N(t) \exp\left(\frac{i\mathcal{A}_R^c}{\hbar} + \frac{imc^2 t}{\hbar}\right). \qquad (26)$$

This result is true but only in an approximate sense to the leading order; the actual propagator for a particle in relativistic quantum theory turns out to be more complicated. This is because the action in (24) for the relativistic particle is not quadratic and our previous result

It is the second interpretation which makes contact with optics so clear and is lacking when we do non-relativistic quantum mechanics.

in (18) does not hold. But, to the leading order, all of it hangs together very nicely. The phase of the propagator is indeed the value of the classical action divided by $\hbar$ and it is also given by the ratio of the spacetime interval between the events and the Compton wavelength. It is the second interpretation which makes contact with optics so clear and is lacking when we do non-relativistic quantum mechanics.

There is actually a valid mathematical reason for this to happen which can be described qualitatively as follows: The Schrödinger equation describing the non-relativistic particle involves first derivative with respect to time but second derivative with respect to spatial coordinates. This works in non-relativistic mechanics in which time is special and absolute. In contrast, in relativistic theories, we treat time and space at a more symmetric footing and use a wave equation in which second derivatives with respect to time also appear. The solutions to such an equation with allow propagation of amplitudes both forward and backward in time coordinate just as it allows propagation both forwards and backwards in spatial coordinates. *When one takes the non-relativistic limit of the field theory, we select out the modes which only propagate forward in time.* This is exactly in analogy with paraxial optics we studied in the last installment. The basic equation for electromagnetic wave will allow propagation in both positive z-direction as well as negative z-direction. But, when we consider a specific context of paraxial optics (for example, a beam of light hitting a couple of slits in a screen and forming an interference pattern or light propagating through a lens and getting focused), we select out the modes which are propagating in the positive z-direction. It is therefore no wonder that the propagator in non-relativistic quantum mechanics is mathematically identical to that in paraxial optics!

Address for Correspondence
T Padmanabhan
IUCAA, Post Bag 4
Pune University Campus
Ganeshkhind
Pune 411 007, India.
Email:
paddy@iucaa.ernet.in
nabhan@iucaa.ernet.in