Snippets of Physics

22. Wigner's Function and Semi-Classical Limit

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.

Obtaining the classical limit of quantum mechanics turns out to be conceptually and operationally non-trivial and, even today, some of the experts consider this issue to be unsettled. There is a function, originally devised by Wigner, which plays a key role in this aspect and throws some light on the way the classical world emerges from the quantum description.

Quantum physics is nothing like classical physics and it is probably not an exaggeration to say that we just get used to quantum physics, without really understanding it, as we learn more about it! There are several conceptual and technical problems involved in taking the classical limit of a quantum mechanical description and we will concentrate on one particular aspect in this installment. We will not worry too much about the conceptual issues – however interesting they are – but will, instead, concentrate on certain technical aspects.

Let us begin with a simple one-dimensional problem in quantum mechanics in which a particle of mass M evolves under the influence of a potential $V(Q)$. Classically, such a system is described by the action functional

$$A = \int L\, \mathrm{d}t; \qquad L = \frac{1}{2} M \dot{Q}^2 - V(Q)\ . \tag{1}$$

The equations of motion can be obtained by varying this action with respect to the coordinate and we get $\ddot{Q} + V'(Q) = 0$. We also know that the system can be equivalently described using the Hamiltonian $H(P,Q) = (P^2/2M) + V$ and the Hamilton–Jacobi equation for the

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system is given by

$$\frac{\partial A}{\partial t} + H\left[\frac{\partial A}{\partial Q}, Q\right] = 0 \qquad (2)$$

which is solved by the action, treated as a function of the variables at upper limit of integration in (1). When we solve the equations of motion we typically obtain the trajectory of the particle $Q(t)$ from which we can obtain the momentum $P(t) = M\dot{Q}(t)$. Given $Q(t)$ and $P(t)$ we can determine the functional form $P = P(Q)$ thereby obtaining the trajectory of the particle in the phase space. (This is, of course, unique only locally, since in general, e.g., for periodic motions, one will be led to multiple- valued functions.) The trajectory in the phase space tells you that you can assign to the particle a position Q and momentum P simultaneously.

Let us move on to quantum theory. Since uncertainty principle prevents our assigning simultaneously the position and momentum to a particle, we can no longer describe the system in terms of a trajectory either in real space or in phase space. Instead we have to invoke a probabilistic interpretation and describe the quantum state of the system in terms of a wave function ψ. This wave function satisfies the standard Schrodinger equation

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial Q^2} + V(Q)\psi = E\psi\ , \qquad (3)$$

where the second equality holds if we are interested in stationary states with the time evolution described by the factor $\exp(-iEt/\hbar)$. For the sake of simplicity, we shall assume that this is the case. We also know that the classical behaviour – trajectories and all – has to emerge from this equation in the limit of $\hbar \to 0$. The question is: How do we go about taking this limit?

It is worth thinking about this issue a little bit before jumping on to the standard text book description. The Schrödinger equation in (3) is a differential equation with $\hbar$ appearing as a parameter. If you haven't read textbooks, you might have thought that one would expand ψ in a Taylor series in $\hbar$ like $\psi = \psi_0 + \hbar\psi_1 + \hbar^2\psi_2$ ..., plug it into the equation and try to solve it order by order in $\hbar$. The $\psi_0, \psi_1 \cdots$ will all have weird dimensions since $\hbar$ is not dimensionless; this, however, is not a serious issue. The key point is that, in such an expansion, we are assuming ψ to be analytic in $\hbar$ with ψ_0 describing the classical limit. This idea, however, does not work, as you can easily verify. In fact, we would have been in a bit of trouble if it had worked since we will then have to interpret ψ_0 as some kind of 'classical' wave function. The way one obtains classical limit is fairly non-trivial which we will now describe.

We will begin by writing the wave function in the form

$$\psi(Q) = R(Q)\exp[iS(Q)/\hbar] \tag{4}$$

which is just the standard representation of a complex number in terms of the amplitude and phase. Substituting into (3) and equating the real and imaginary parts, we get the two equations

$$(R^2 S')' = 0 \ , \tag{5}$$

and

$$\frac{S'^2}{2M} + V(Q) - E = \frac{\hbar^2}{2M}\frac{R''}{R} \ . \tag{6}$$

These two equations can be manipulated to give a single equation for S (when $S' \neq 0$). We get

$$\frac{S'^2}{2M} + V(Q) - E = \frac{\hbar^2}{2M}\sqrt{S'}\left[\frac{\mathrm{d}^2}{\mathrm{d}Q^2}[1/\sqrt{S'}]\right] \ . \tag{7}$$

The Schrödinger equation is completely equivalent to the two real equations in (5) and (6). Anything you can do with a complex wave function ψ you can also do with two real functions R and S. But, of course, Schrödinger equation is linear in ψ while equations (5) and (6) are nonlinear, thereby hiding the principle of superposition of quantum state, which is a cornerstone of quantum description.

Equation (7) suggests an alternate route for doing the Taylor series expansion in $\hbar$. We can now try to interpret the left-hand side of (7) as purely classical and the right-hand side as giving 'quantum corrections'. In such a case, we can attempt a Taylor series expansion in the form

$$S(Q) = S_0(Q) + \hbar^2 S_1(Q) + \cdots \ . \tag{8}$$

This means that the leading behaviour of the wave function is given by $\exp(iS_0/\hbar)$ which is *non-analytic* in $\hbar$. It does not have a Taylor series expansion in powers of $\hbar$ which is a different kettle of fish when it comes to series expansion in terms of a parameter in a differential equation. Also note that the time-*independent*

Schrödinger equation depends only on $\hbar^2$ and not on $\hbar$; so the second term in the Taylor series starts with $\hbar^2$ and not with $\hbar$.

Why does this approach work while $\psi = \psi_0 + \hbar\psi_1 + \hbar^2\psi_2$ ..., does not lead to sensible results? The reason essentially has to do with the fact that, in proceeding from quantum physics to classical physics, we are doing something analogous to obtaining the ray optics from electromagnetic waves. One knows that this can come about only when the phase of the wave is non-analytic in the expansion parameter, which is essentially the wavelength in the case of light propagation. So you need to bring in some extra physical insight to obtain the correct limit.

While ψ is non-analytic in $\hbar$, we have now translated the problem in terms of R and S which are (assumed to be) analytic in $\hbar$ so that the standard procedure works. To the leading order, we will ignore the right-hand side of (7) and obtain the equation

$$\frac{S_0'^2}{2M} + V(Q) - E = 0\ . \tag{9}$$

(This might seem pretty obvious but there is a subtlety lurking here which we will comment on later.) To the same order of accuracy, we find that $R(Q) \propto |S_0'(Q)|^{-1/2}$. Putting it together and noting the fact the two independent solutions will involve $\pm S_0'$, we can write the solution to the Schrödinger equation to this order of accuracy by

$$\psi_E^{(0)} = \frac{1}{\sqrt{|S_0'|}}\left[C_1 \exp\left[\frac{i}{\hbar}S_0(Q)\right] + C_2 \exp\left[-\frac{i}{\hbar}S_0(Q)\right]\right]\ , \tag{10}$$

where C_1 and C_2 are arbitrary constants. To this order of accuracy, the (9) is just the Hamilton–Jacobi equation for the action $A = S_0$ so that we can identify the phase of the wavefunction with $S_0/\hbar$. The condition of validity for this WKB approximation is not difficult to determine by comparing the terms which were ignored with those which were retained. We find that this condition is equivalent to

$$\hbar\left|\frac{S''}{S'^2}\right| = \left|\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\hbar}{S'}\right)\right| \ll 1 \tag{11}$$

which translates to

$$2M\hbar|V'| \ll (2M[E - V(Q)])^{3/2}\ . \tag{12}$$

So, as long as we are far away from the turning points in the potential (where $E = V(Q)$), one can satisfy this condition.

Though we approached this result from a desire to obtain the classical limit, mathematically speaking, it is just an approximation to the differential equation usually known as WKB approximation. This fact is strikingly evident in the context of quantum mechanical tunneling which, of course, has no classical analogy. Nevertheless, we can get a reasonable approximation to the wave function in a classically forbidden form by taking $E < V(Q)$ in (9). In this range, say, $a < Q < b$ in which $E < V(Q)$, the S_0 becomes purely imaginary and is given by

$$S_0 = \sqrt{2M}\int_a^b \sqrt{E - V(Q)}\ \mathrm{d}Q = i\sqrt{2M}\int_a^b \sqrt{V(Q) - E}\,\mathrm{d}Q. \tag{13}$$

The wave function in (10) becomes exponentially decreasing (or increasing) – without oscillatory behaviour – in this classically forbidden range. This is valid, again, as long as we are away from the turning point.

Let us now get back to the question we started with, viz., how to get the classical limit. To do this we need to understand why the wave function in (10) has anything to do with the classical limit. The conventional answer is as follows: Let us consider for simplicity a situation with $C_2 = 0$. In that case the probability distribution associated with the wave function varies as

$$\mathcal{P} \equiv |\psi|^2 \propto \frac{1}{P(Q)}\ , \tag{14}$$

where $S_0'(Q) = P(Q)$ is the *classical* momentum of the particle at Q. If we now interpret the probability to catch a particle in the interval $(Q, Q + dQ)$ as proportional to the time interval $\mathrm{d}t = \mathrm{d}Q/V(Q)$ (where $V(Q)$ is the velocity of the particle when it is at Q) then the expression in (14) can be given some kind of a classical interpretation. This is, however, not completely satisfactory because, as we said earlier, we associate the classical limit with a deterministic trajectory in phase space. There is a way of obtaining this result which brings us to the discussion of the Wigner function.

The Wigner function $F(Q, p, t)$ corresponding to a wave function $\psi(Q, t)$ (which could, in general, be time dependent) is defined by the relation

$$F(Q, p, t) = \int_{-\infty}^{\infty} \mathrm{d}u\,\psi^*\left(Q - \frac{1}{2}\hbar u, t\right) \mathrm{e}^{-ipu}\psi\left(Q + \frac{1}{2}\hbar u, t\right). \tag{15}$$

The integrand measures the correlation between ψ and ψ^* in a Fourier transformed space with variable p. This function has several remarkable properties which we will now discuss. The basic idea is to see whether one can think of F as a probability distribution function in the phase space with position (Q) and momentum (p) as coordinates.

To begin with, if you integrate F over the momentum variable p, and use the fact that the integral of $\exp(ipu)$ over p is a Dirac delta function in u, you get

$$\int_{-\infty}^{\infty} \mathrm{d}p \ F(Q,p,t) = |\psi(Q,t)|^2 \ . \tag{16}$$

This shows that when marginalized over p, we do get the probability distribution Q which is quite nice. Further, it is also easy to see that if you integrate F over Q you get the result

$$\int_{-\infty}^{\infty} \mathrm{d}Q \ F(Q,p,t) = |\phi(p,t)|^2 \ , \tag{17}$$

where $\phi(p,t)$ is the Fourier transform of $\psi(Q,t)$. From the standard rules of quantum mechanics, we know that $\phi(p,t)$ gives the probability amplitude in the momentum space. Therefore (17) tells us that – when marginalized over the coordinate Q – the Wigner function F gives the probability distribution in the momentum space. So clearly, F satisfies two nice properties we would have expected out of a probability distribution. It simultaneously encodes both coordinate space and momentum space probabilities in a state represented by ψ.

It is also possible to obtain an equation satisfied by F which is similar to the continuity equation that we expect probability distributions to satisfy. Direct differentiation of (15) and some clever manipulation will allow you to obtain an equation of the form

$$\frac{\partial F}{\partial t} + \frac{p}{M}\frac{\partial F}{\partial Q} - \frac{\mathrm{d}V}{\mathrm{d}Q}\frac{\partial F}{\partial p} = \frac{\hbar^2}{24}\frac{\mathrm{d}^3 V}{\mathrm{d}Q^3}\frac{\partial^3 F}{\partial p^3} + \cdots \ , \tag{18}$$

where $\cdots$ denotes terms which are higher order in $\hbar$. This equation allows you to draw two interesting conclusions. To begin with, if the potential is at most quadratic in coordinates, the right-hand side vanishes and we get exactly the continuity equation in the phase space with the semi-classical identifications

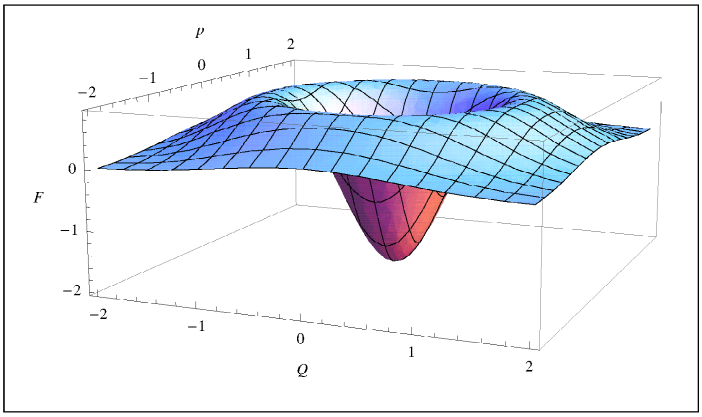

Figure 1.

$\dot{Q} = p/m$ and $\dot{p} = -V'$. Next, this interpretation holds even for *arbitrary* potentials up to linear order in $\hbar$. If we can ignore the $\hbar^2$ in the right-hand side we again get the continuity equation in phase space.

Before we rejoice, one has to face up to a rather damaging property of F which prevents us from making the probabilistic interpretation rigorous. The key trouble is that F is not positive definite and since we do not know how to interpret negative probabilities, we cannot use F as a probability distribution in phase space. One simple way to see that F can become negative is to compute it for some well-chosen state. For example, *Figure* 1 gives the Wigner function corresponding to the first excited state of a harmonic oscillator. We have, in suitably chosen units, the results:

$$\psi_1(Q) = \left(\frac{4}{\pi}\right)^{1/4} Q\ e^{-(Q^2/2)}\ ; \qquad (19)$$

$$F(Q,p) = 4\left(Q^2 + p^2 - \frac{1}{2}\right) e^{-(p^2+Q^2)}\ . \qquad (20)$$

It is clear that F can go negative.

This does not, however, prevent us from using the Wigner function in suitable limits as an approximation to classical probability distribution. In particular, the Wigner function corresponding to the semi-classical wave function in (10) is quite easy to interpret. Let us first consider the case with $C_2 = 0$ when the wave function becomes

$$\psi(Q) = \left(\frac{C_1}{\sqrt{S_0'}}\right) \exp(iS_0/\hbar)\ . \qquad (21)$$

Substituting this into (15) and evaluating the integrals – retaining up to the correct order, which is necessary since ψ itself is approximate – we can easily show that

$$F(Q,p) = \frac{|C_1|^2}{|S_0'(Q)|}\delta\left(p - \frac{\partial S_0}{\partial Q}\right) + \mathcal{O}(\hbar^2) \ . \tag{22}$$

This result, when we think of F as a probability distribution, has a nice interpretation. The Dirac delta function tells you that when the particle is at Q, its momentum is sharply peaked at $\partial S_0/\partial Q$ which is exactly what we would have expected if the particle was moving along a classical trajectory. Further, the probability to find the particle around Q is proportional to $(1/S'(Q))$ which again can be interpreted in terms of the time $\mathrm{d}t = \mathrm{d}Q/V(Q)$ which the particle spends in the interval $(Q, Q + \mathrm{d}Q)$.

The key point is that, for the semi-classical wave function we determined in (10), the Wigner function gives strongly correlated probability distribution in phase space. In fact, if you take the Dirac delta function literally, it gives a unique p for every Q. This is the characteristic of a classical trajectory and, from this point of view, the Wigner function provides a natural interpretation for the semi-classical wave function we have obtained. Note that the probability distribution is not peaked around any single trajectory but once you pick a Q, it gives you a unique p. This correlation between momentum and position is the key feature of classical limit. This interpretation continues to hold even when we keep $C_2 \neq 0$. In this case we get

$$F(Q,p) = \frac{|C_1|^2}{|S_0'(Q)|}\delta\left(p - \frac{\partial S_0}{\partial Q}\right) + \frac{|C_2|^2}{|S_0'(Q)|}\delta\left(p + \frac{\partial S_0}{\partial Q}\right) + \mathcal{O}(\hbar^2) \ . \tag{23}$$

The Wigner function has a term which represents interference between the two independent solutions but this term is $\mathcal{O}(\hbar^2)$ and does not contribute at the leading order. This Wigner function is now peaked at two different values of momenta $p = \pm\partial S_0/\partial Q$ and corresponds to motion along forward and backward direction in the coordinate space. In the phase space, F will now be peaked on two families of trajectories.

These properties are obviously special to the semi-classical wave function we have chosen. If you take a classically forbidden region in which the wave function is exponentially damped, rather than oscillatory, you will find a completely different behaviour for the Wigner function. In fact, in such a 'purely quantum mechanical' situation, you will find that the Wigner function factorizes into a product of two functions, one dependent on Q and the other dependent on p with $F(Q,p) = F_1(Q)F_2(p)$. This shows that the momentum and position are totally uncorrelated in such a state which clearly is the other extreme of the semi-classical state in which the momentum is completely correlated with position.

The same decoupling of momentum and position dependence occurs for many other states. One simple example is the ground state of the harmonic oscillator for which you will find that the Wigner function factorizes into two products, both Gaussian in position and momentum. So the ground state of the harmonic oscillator is as non-classical as a state could get in this interpretation.

Finally, let us get back to the subtlety which I mentioned earlier in ignoring the right-hand side of (6) which is a closely related issue. For this approximation to be valid, we must have

$$\lim_{\hbar\to 0} \frac{\hbar^2}{2M}\frac{R''}{R} = 0 \ . \tag{24}$$

It is easy to construct states for which this condition is violated! As a simple example, consider the ground state of a system in a bounded potential which will be described by a real wave function. In this case $\psi = R$ and $S = 0$. From (6) we now see that

$$\frac{\hbar^2}{2M}\frac{R''}{R} = V(Q) - E \ . \tag{25}$$

The limit in (24) cannot now hold, in general. Clearly our analysis fails for the ground state of a quantum system. To see this explicitly, consider again the ground state of a harmonic oscillator:

$$\psi(Q) = N \exp\left[-\frac{M\omega}{2\hbar}Q^2\right] \ . \tag{26}$$

Being an exact solution to the Schrödinger equation the amplitude and phase (which is zero) of this wave function satisfies (5) and (6). A straightforward computation now shows – not surprisingly – that

$$\frac{\hbar^2}{2M}\frac{R''}{R} = \frac{1}{2}M\omega^2 Q^2 - \frac{1}{2}\hbar\omega \ . \tag{27}$$

When we take the limit $\hbar \to 0$, the second term on the right-hand side vanishes but not the first term! This means there are quantum states for which we cannot naively take the right-hand side of (6) to be zero and determine the classical limit. Interestingly enough, this is also true for the time-dependent, coherent states of the oscillator. You may want to amuse yourself by analyzing this situation in greater detail.

Suggested Reading

[1] **Some of the pedagogical details regarding Wigner functions can be found in the article, W B Case, *Am. J. Phys.*, Vol.76, p.937, 2008.**

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

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