Quantum mechanics, macroscopic objects, and the classical limit

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Some of the recent discussions on RG displayed a substantial lack of knowledge regarding the current status of certain physical theories, so it may be time for some teaching about a few issues, in order to reestablish a basis on which to ground a *meaningful* discussion. There is no point in arguing with a view that has been known to be erroneous for well beyond fifty years.

I suppose I am qualified to fill in a few of the knowledge gaps, having taught quantum mechanics since 1997; not every year, but every other year on average. In addition, I have taught quantum statistical physics about as often. Further, I have given a smaller number of courses on elements of relativistic quantum mechanics and field quantization. So, I believe to know my basics.

Applicability of quantum mechanics to macroscopic systems

First, the idea should be debunked that quantum mechanics cannot be applied to macroscopic objects. Statistical mechanics is the physical theory dealing with macroscopic objects, and quantum statistical mechanics is the theory doing the same on the basis of quantum mechanics. And it is a well-established theory.

Apparently, the error seems to be largely based on the belief that a wave function cannot be assigned to a macroscopic body. Which is not true in all cases, as one *can* describe superconductivity and superfluidity using macroscopic wave functions (whose wave length is not the de Broglie wave length of the macroscopic body), but the main argument to be made here is that quantum mechanics is not mainly about wave functions or interference. In fact, *classical* electrodynamics describes electromagnetic radiation as a *wave phenomenon*, and this description is confirmed by Young's double slit experiment. What quantum mechanics *adds* is the fact that electromagnetic radiation *cannot* always be so described and that there are *photons*, behaving as *particles*.

The state of a macroscopic body is given, in the large majority of cases, by a density operator. Density operators are a mathematical tool to capture both coherent and incoherent superpositions of states. And of course, quantum mechanics is not just wave mechanics. In statistical mechanics, the quantum state is, due to the fact that macroscopic systems are open systems rather than closed ones,[1] almost never a pure state. Nevertheless, a classical statistical description would lead to disagreement with observations.

A few examples may be in order.

The one I like most is magnetism. We have the Bohr-van Leeuwen theorem, stating that in classical physics, a macroscopic body in thermodynamic equilibrium cannot display magnetism. This is a rigorous statement, following from the form of the partition function in classical statistical mechanics. Therefore, diamagnetism, paramagnetism, and ferromagnetism are all quantum phenomena and, what is more, *macroscopic* quantum phenomena. To explain them, we *need* quantum statistical mechanics, as classical statistical mechanics states their *absence*, a rigorous and exact result... But not applicable to the real world, because the real world is *not* classical. Note that both the theorem and quantum mechanics exempting from it are

[1] They may exchange energy with the environment at the microscopic scale, even when a strong attempt is made to keep the system isolated.

talking about macroscopic bodies, because of the requirement of thermodynamic equilibrium (which is meaningless for a microscopic body).

Another example is black-body radiation. The spectral energy density $u(\omega, T)$ for black-body radiation can be derived rigorously within classical physics.[2] The result is

$$u(\omega, T) = \frac{\omega^2}{\pi^2 c^3} k_B T \,, \tag{1}$$

where ω is the (angular) frequency of the radiation, T the temperature, c the speed of light, and k_B is Boltzmann's constant. This is the Rayleigh-Jeans formula. Unfortunately, if you integrate it over all frequencies, this *exact* formula produces an *infinite* total energy density, a phenomenon that was termed ultraviolet catastrophe.

Quantum mechanics comes to the rescue. Planck gave a somewhat heuristic derivation, justified essentially by the fact that it worked, quantum mechanics not yet having been invented. Nowadays, we know how to do things properly in quantizing the electromagnetic field and then carrying out discrete sums involving the partition function. The result is of course Planck's formula:

$$u(\omega, T) = \frac{\omega^2}{\pi^2 c^3} \frac{\hbar\omega}{\mathrm{e}^{\hbar\omega/k_B T} - 1} \,, \tag{2}$$

and this correctly describes even the cosmic background radiation, which hardly can be called a microscopic system. Note also that we may take the limit $\hbar \to 0$ in Eq. (2); de l'Hospital's rule gives for the second factor $\lim_{\hbar\to 0} \frac{\omega}{(\omega/k_B T)\mathrm{e}^{\hbar\omega/k_B T}} = k_B T$, so we recover the Rayleigh-Jeans formula (1), the classical limit.

There are many other macroscopic systems or phenomena that can only be correctly described by quantum mechanics. Besides superconductivity (including Josephson effects) and superfluidity, there is the specific heat of a macroscopic body, which classical statistics predicts to be constant, whereas quantum mechanics correctly describes its tending to zero as $T \to 0$. There are also really massive bodies that we can describe only based on quantum mechanical results – neutron stars. They owe their mere existence to the fact that there is a degeneracy pressure in the quantum state of the neutrons, despite their thermal pressure being incapable of counteracting the huge gravity present in the system.

Degeneracy pressure is a consequence of the Pauli exclusion principle, valid for fermions. Quantum statistical mechanics takes into account the fact that there are two possibilities for the many-particle wave functions used in the construction of the density operator - they must be either symmetric under particle exchange or antisymmetric, due to the indistinguishability of the particles. In the first case, these are bosons and we may have phenomena such as Bose condensation (again a macroscopic phenomenon), in the second, they are fermions, and then quantum statistics leads to the Pauli exclusion principle and degeneracy pressure.

I think, it is fair to say that without applying quantum mechanics to macroscopic systems, which is regularly done in quantum statistical mechanics, we would be unable to account for a large number of everyday phenomena (magnetism, specific heat) and more exotic phenomena (superconductivity, neutron stars).

[2] The equipartition theorem comes into play.

The classical limit

Second, I would like to demonstrate that classical physics is indeed obtained from quantum mechanics by taking the limit $\hbar \to 0$, a claim that was contested here several times.

As shown above, the classical formula (1) for black-body radiation results from the quantum mechanical one (2) via this limit, which may serve as an example.

Since it seems necessary due to the "quality" of some of the objections, let me first discuss what it means mathematically to take a limit and then what ramifications there are in physics.

In mathematics, the meaning of

$$\lim_{x \to x_0} f(x) = c$$

is precisely defined and given by

$$\forall \varepsilon > 0 \quad \exists \delta > 0 \quad \text{so that} \quad |f(x) - c| < \varepsilon \quad \forall x \quad \text{satisfying} \quad |x - x_0| < \delta \, .$$

This definition in terms of "epsilontics" is the one typically used when trying to establish a limit rigorously. It should be clear that the idea of x "moving" versus x_0 and at the same time $f(x)$ "moving" versus c is a useful visualization of the limiting process but nothing more. We may consider the limit of a function of x for $x \to x_0$ whether x is really a varying quantity or not. If x is a constant that happens to be close to x_0, the value of the limit may still be useful.

A physically interesting example is the standard derivation of the Casimir effect, where ideally conducting metal plates are assumed, which makes the effect material independent [1]. This means assuming the Sommerfeld fine structure constant α to be large compared with some quantity involving the inverse plasma frequency. The final formula for the Casimir effect corresponds to the limit of taking the Sommerfeld fine structure constant to infinity! In reality, $\alpha \approx 1/137$, which is small for many purposes but large in the context discussed (where it is compared with a quantity that is typically of the order of 10^{-5}). Of course, there would be no Casimir effect, if the fine structure constant were zero.

The fine structure constant is nondimensional, so it is possible to immediately apply the mathematical definition when exploring a limit. There is an additional twist, when limits of dimensional quantities are to be considered, which is the case for $\hbar$. Dimensional quantities cannot be said to be large or small except in comparison with another quantity of the same dimension. Theorists like to set certain dimensional quantities such as $\hbar$, c or G equal to one to simplify formulas. There is no magic involved – this simply means measuring actions in units of $\hbar$, velocities in units of c and, e.g., the Schwarzschild radius in units of a mass. We are free to choose our units. But clearly, we cannot consider a quantity small or large that we have set equal to one by a choice of unit. Instead, if we wish to consider the limit $\hbar \to 0$, we should consider the ratio of $\hbar$ and some action or of $\hbar\omega$ and some energy, with the second quantity being large with respect to $\hbar$ or $\hbar\omega$. This is the standard meaning of a classical limit, because classical actions are typically large compared with $\hbar$ and classical energies large compared with the energy of a single photon. So the meaning of taking the limit of $\hbar \to 0$ simply is taking the limit of $\hbar/S \to 0$, where S is some appropriately chosen quantity with the dimension of an action [$k_B T/\omega$ in the case of formula (2)]. Obviously, the fact that $\hbar$ is a constant then does not play any role at all, because S need not be constant.

Reconsider now Eq. (2). If taking the limit $\hbar \to 0$ actually means finding a dimensionless quantity involving $\hbar$ that goes to zero, what would be a natural choice? Why, the argument

of the exponential must be dimensionless, so we may choose $x = \hbar\omega/k_BT$ as dimensionless variable, rewrite the formula as

$$u(\omega, T) = \frac{\omega^2}{\pi^2 c^3} k_B T \frac{x}{\mathrm{e}^x - 1} \,, \tag{3}$$

and take the limit $x \to 0$, which of course gives Eq. (1) again. But we gain two new interpretations of the classical limit. Taking $x \to 0$ can be achieved by sending $\omega \to 0$ (i.e., $\omega \ll k_BT/\hbar$) or $T \to \infty$ (i.e., $T \gg \hbar\omega/k_B$), so the classical limit is the limit of either low frequencies or high temperatures. Note that contrary to the limit $\hbar \to 0$ which can be carried out on the full formula (2), these two other limits should only be performed on the factor involving x, in order not to make the whole result equal to 0 or ∞. We talk of the asymptotic behavior of the formula for small ω or large T rather than of its limit in this case. Asymptotic behaviors may include more information than just the limit result (which would be the vanishing of u for $\omega \to 0$ and its divergence for $T \to \infty$) or just the leading order behavior.

Now the creators of quantum mechanics made it explicit that their theory reduces to classical mechanics in the limit $\hbar \to 0$. This simply was a consistency check for them. Quantum mechanics was from the outset devised as an extension of classical mechanics to the microscopic domain, but, as in all extensions of theories before,[3] the intention was not just to produce a theory for the new domain of application (atoms in the case of quantum mechanics). No, the point was to create a theory that encompasses the old theory but is valid beyond the classical domain. Quantum theory is not a theory of microscopic systems (alone). It was devised as a theory of atomic spectra that also covers the classical domain (and intermediate cases such as Rydberg atoms). Bohr expressed this in terms of his correspondence principle, and Feynman, the author of the third formulation of quantum mechanics writes in his thesis [2] on p. 27: *"Classical mechanics is the limiting form of quantum mechanics, when Planck's constant, ħ, is considered being vanishingly small. The classical system analogous to a quantum mechanical system (when such an analogy exists) may be mathematically exhibited most directly by letting ħ approach zero in the quantum mechanical equations."*

Now in physics, contrary to the humanities and other "non-exact" sciences, we need not rely on authorities. We need not take Feynman's nor Bohr's word for checking the statement that classical mechanics arises as a limiting case of quantum mechanics and therefore is contained in it. We can ourselves check the mathematical proofs that are offered for a statement (of course, we must have a certain level of mathematical competence to do so, but otherwise, physics allows minds to free themselves from "truths by decree").

Therefore, I will simply sketch the mathematical approaches demonstrating classical mechanics being the limit of quantum mechanics as $\hbar \to 0$, for the three known formulations of quantum mechanics. These sketches can be fleshed out into rigorous proofs by anyone with sufficient mathematical competence. So if you are left in doubt by my outline, you are free to study the question in more detail in the literature, which may require that you first increase your mathematical skills. Of course, it would be sufficient to study the question in a single formulation of quantum mechanics. But since the case is extremely simple in the Schrödinger picture and Feynman gives a proof for his formulation of quantum mechanics himself, I might as well provide all three approaches. I will restrict myself to considering a single particle – the generalization to many-particle systems is straightforward, as long as the particle number is fixed.

[3]For example, special relativity and general relativity are extensions of Newtonian mechanics and Newtonian gravity that are valid not only for large velocities and large gravitational fields but also for small ones.

Schrödinger picture

The Schrödinger equation in position representation is

$$\mathrm{i}\hbar\frac{\partial\psi(\boldsymbol{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t)\,. \tag{4}$$

To simply set $\hbar$ equal to 0 in the equation is problematic, because the only surviving term would be the last one, stating that $\psi(\boldsymbol{x},t)$ must be zero everywhere except where $V(\boldsymbol{x}) = 0$. While a δ function limit for ψ would not seem unreasonable, it does not make much sense that the peaks of this δ function fall onto the zeros of V. In fact, setting $\hbar = 0$ reduces the order of the differential equation, even turning it into an algebraic equation, which destroys the general solution structure. This phenomenon is known from other examples. Whenever a small factor multiplies the highest derivative in a differential equation, the order of the equation is reduced on setting that "perturbation" equal to zero, meaning that the solution of the "unperturbed" equation depends on fewer constants of integration than that of the perturbed one. For linear equations, the number of fundamental solutions is reduced. Therefore, the solution space must change – increasing its dimension – when the perturbation is "switched on". Such a perturbation that alters the solution space itself (rather than only the solutions) is called a *singular* perturbation. It may even happen that the unperturbed problem has no solution at all while the perturbed one is solvable (and vice versa). Methods have been developed to deal with singular perturbations. They belong to the field of asymptotic analysis, on which I have given courses even more often than on quantum mechanics.

When a singular perturbation appears, it is important to distinguish between the problem without perturbation and the zeroth order of the perturbed problem. They do not usually have the same solutions. In the case of quantum mechanics, singular perturbation theory runs under the name of WKB(J) theory, applicable to the semiclassical limit. We will look at a somewhat simpler approach, since we are interested in the classical limit, not just the semiclassical one, where a wave function is still calculated. In the fully classical limit, we do not care about the breakdown of a wave function solution – we want to get trajectories.

The first step is to rewrite the wave function in terms of a real amplitude factor and a phase:

$$\psi(\boldsymbol{x},t) = A(\boldsymbol{x},t)\exp\left(\frac{\mathrm{i}}{\hbar}S(\boldsymbol{x},t)\right)\,. \tag{5}$$

Here $S(\boldsymbol{x},t)$ is a real function, too. It must have the dimension of an action for the exponent to remain dimensionless. $\hbar$ has been put in the denominator in order to capture any fast variations that the wave function may develop in the limit $\hbar \to 0$. Then $S(\boldsymbol{x},t)$ need not vary fast itself. Moreover $A(\boldsymbol{x},t)$ varies slowly, too, as the calculations reveal. Note that we would not have to write a prefactor $A(\boldsymbol{x},t)$ at all, if we allowed $S(\boldsymbol{x},t)$ to become complex.[4]

Inserting (5) into the Schrödinger equation and separating real and imaginary parts, we get two equations

$$\frac{\partial A(\boldsymbol{x},t)}{\partial t} = -\frac{1}{2m}\left\{A(\boldsymbol{x},t)\nabla^2 S(\boldsymbol{x},t) + 2\nabla A(\boldsymbol{x},t)\nabla S(\boldsymbol{x},t)\right\}\,, \tag{6}$$

$$\frac{\partial S(\boldsymbol{x},t)}{\partial t} = -\left\{\frac{(\nabla S(\boldsymbol{x},t))^2}{2m} + V(\boldsymbol{x}) - \frac{\hbar^2}{2m}\frac{\nabla^2 A(\boldsymbol{x},t)}{A(\boldsymbol{x},t)}\right\}\,. \tag{7}$$

[4]This is often done in WKB theory. But interpretations are simpler, if we keep a real amplitude and a real phase explicitly.

These are still exact, i.e., they represent just a rewriting of the Schrödinger equation in a different form. Note that the last term in Eq. (7) is the famous quantum potential introduced by Bohm [3]. The name is appropriate, as the term adds to the ordinary potential and vanishes, if $\hbar$ is sent to zero.

In fact, the reformulation (6) and (7) of the Schrödinger equation is much better suited for taking that limit than the original form, because now the pair of equations remains a set of differential equations. Dropping the quantum potential in (7), we obtain

$$\frac{\partial S(\boldsymbol{x},t)}{\partial t} + \frac{(\nabla S(\boldsymbol{x},t))^2}{2m} + V(\boldsymbol{x}) = \frac{\partial S(\boldsymbol{x},t)}{\partial t} + H(\nabla S(\boldsymbol{x},t),\boldsymbol{x}) = 0\,, \tag{8}$$

where $H(\boldsymbol{p},\boldsymbol{x})$ is the classical Hamiltonian. To those among you who know their classical mechanics well, the demonstration may already look complete, because Eq. (8) is simply the Hamilton-Jacobi equation, one of the formulations of classical Hamiltonian mechanics, from which the solution of the classical problem governed by the Hamiltonian $H(\boldsymbol{p},\boldsymbol{x})$ can be obtained by finding a solution depending on three *nontrivial* constants of integration for $S(\boldsymbol{x},t)$.[5] The momentum is given by $\boldsymbol{p} = \nabla S$. For those who are less familiar with the Hamilton-Jacobi formalism, the latter result may be gathered from Eq. (6). Multiplying it by A and remembering that $A^2(\boldsymbol{x},t) = |\psi(\boldsymbol{x},t)|^2 \equiv w(\boldsymbol{x},t)$ is the probability density for position measurements, we find

$$\frac{\partial w(\boldsymbol{x},t)}{\partial t} + \nabla\cdot\left(\frac{\nabla S}{m}w(\boldsymbol{x},t)\right) = 0\,, \tag{9}$$

which is a continuity equation, from which we immediately infer that $\frac{\nabla S}{m}$ is the particle velocity.

Since the Hamilton-Jacobi equation is equivalent to Hamilton's equations of motion, we obtain trajectories of particles from it, if the initial condition is determinate. That is, we have to supplement Eq. (8) with an initial position and momentum of the particle to obtain a definite solution. Heisenberg's uncertainty relation $\Delta p_i \Delta x_i > \hbar/2$ prevents us from specifying precise values for position and momentum (components along one coordinate direction) simultaneously. However, since the relation expresses the fluctuations of position and momentum in terms of $\hbar$, it does not impose any restrictions in the limit $\hbar \to 0$. Therefore, it is possible to specify sharp initial conditions in that limit. Then $w(\boldsymbol{x},0)$ is a δ function and Eq. (9) tells us that the probability density will remain a delta function, the peak of which is advected with the velocity $\nabla S/m$, i.e., we have $w(\boldsymbol{x},t) = \delta\left(\boldsymbol{x}_{\rm cl}(t) - \boldsymbol{x}\right)$, where $\boldsymbol{x}_{\rm cl}(t)$ denotes the trajectory.

Clearly, in real systems, the limit $\hbar \to 0$ is not exactly achieved, because the classical action with which $\hbar$ is to be compared, never is infinite. Therefore, there will remain a small indeterminacy of the initial conditions, hence $w(\boldsymbol{x},t)$ will become a true probability distribution, widening in the course of time. So will quantum mechanics always make itself felt in classical systems, if only we wait long enough? Not necessarily. Classical systems typically have many degrees of freedom, and the generic behavior of the (normally nonlinear) equations of motion is chaotic. Therefore, there may be sufficient disorderly behavior for the deterministic system to completely dominate the quantum behavior at all times.

Whether or not the limit is exactly achieved in real systems is of course irrelevant for the theoretical question whether classical mechanics is contained in quantum mechanics or not,

[5] Which turns out to be the classical action $S(\boldsymbol{x},t) = \int_{t_0}^{t} L(\boldsymbol{x}(t'),\dot{\boldsymbol{x}}(t'),t')\mathrm{d}t'$, L being the classical Lagrangian. There is always a *trivial* additive constant of integration, because with S also $S+$ const. solves the Hamilton-Jacobi equation.

a question that we have just answered in the affirmative (for all Hamiltonian one-particle systems).

What happens to the wave function in the limit $\hbar \to 0$? Equation (5) obviously suggests that it does not have a well-defined limit.[6] Note that we would not have to worry about the divergence of the phase, if S were a constant, because a global phase factor of the wave function does not affect physical results and could be "renormalized away". However, $S(\boldsymbol{x})$ is not normally constant, so the wave function oscillates in space and these oscillations get more violent (their frequency increases) as $\hbar$ gets smaller.

There may be quantum systems that do not have a classical limit. However, this is not in conflict with our general statement saying that each classical system is the limit of a quantum one. The converse need not be true. The set of classical systems is contained in that of quantum systems but not vice versa.

Heisenberg picture

From the responses I got to my earlier discussion of the Heisenberg picture and the Ehrenfest theorem, it is apparent that the operator relations of this picture have not been understood by some members of the audience. Moreover, strange ideas were voiced such as an acceleration operator not being defined in quantum mechanics.[7] Therefore, I will try to go slowly here and give appropriate explanations of every relevant detail. Also, I will, in this section, notationally distinguish the position and momentum operators by putting a hat on top of their symbols, so as to make clear where we are dealing with operators and where we have eigenvalues or expectation values.

Let us start with the definition of an operator corresponding to an observable in the Heisenberg picture. We have

$$B(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}H(t-t_0)} B_S \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t-t_0)} \,, \tag{10}$$

where B_S is the operator (assumed time-independent here) describing the same observable B in the Schrödinger picture and t_0 is the initial time, e.g. the time of experimental preparation of the system. I will henceforth set t_0 equal to zero. It is straightforward to calculate the time derivatives of a Heisenberg operator. We have

$$\dot{B}(t) = \frac{\mathrm{i}}{\hbar} H \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht} B_S \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} - \frac{\mathrm{i}}{\hbar} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht} B_S \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} H = \frac{\mathrm{i}}{\hbar} \left[H, B(t)\right] \,, \tag{11}$$

$$\begin{aligned} \ddot{B}(t) &= \frac{\mathrm{i}}{\hbar} \left[H, \dot{B}(t)\right] = -\frac{1}{\hbar^2} [H, [H, B(t)]] = \\ &= -\frac{1}{\hbar^2} \left\{ H^2 \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht} B_S \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} - 2H \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht} B_S \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} H + \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht} B_S \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} H^2 \right\} \,. \end{aligned} \tag{12}$$

The equation $\dot{B}(t) = \frac{\mathrm{i}}{\hbar} [H, B(t)]$, derived here from the representation of $B(t)$ in terms of Schrödinger operators is Heisenberg's equation of motion and replaces the Schrödinger equation in the present picture. Obviously, the operators corresponding to arbitrary-order time

[6] The limit is singular. So is the limit of $\left|\psi(\boldsymbol{x}, t)^2\right|$, but it is much more benign, tending to a δ function.

[7] There is an operator associated with *any* classical observable in quantum mechanics (except time), so there is of course an acceleration operator, too.

derivatives of observables can be constructed without any difficulty in the Heisenberg picture.[8]

Next we note that the fundamental commutator relation between momentum and position operators is unchanged in the Heisenberg picture:

$$\begin{aligned}[\hat{p}_j(t), \hat{x}_k(t)] &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\hat{p}_{Sj}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\hat{x}_{Sk}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} - \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\hat{x}_{Sk}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\hat{p}_{Sj}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} \\ &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\,[\hat{p}_{Sj}, \hat{x}_{Sk}]\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}\frac{\hbar}{\mathrm{i}}\delta_{jk}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} = \frac{\hbar}{\mathrm{i}}\delta_{jk}\,. \qquad j,k = 1\ldots 3\,. \end{aligned} \tag{13}$$

This then implies

$$\begin{aligned}[\hat{p}_j, \hat{x}_k^n] &= \frac{\hbar}{\mathrm{i}}\delta_{jk}\,n\hat{x}_k^{n-1} = \frac{\hbar}{\mathrm{i}}\delta_{jk}\,\frac{\partial \hat{x}_k^n}{\partial \hat{x}_k} = \frac{\hbar}{\mathrm{i}}\,\frac{\partial \hat{x}_k^n}{\partial \hat{x}_j}\,, \\ \left[\hat{x}_k, \hat{p}_j^n\right] &= -\frac{\hbar}{\mathrm{i}}\delta_{jk}\,n\hat{p}_j^{n-1} = -\frac{\hbar}{\mathrm{i}}\delta_{jk}\,\frac{\partial \hat{p}_j^n}{\partial \hat{p}_j} = -\frac{\hbar}{\mathrm{i}}\,\frac{\partial \hat{p}_j^n}{\partial \hat{p}_k}\,, \end{aligned} \tag{14}$$

where I have suppressed the time argument for brevity (each operator is a function of t). These formulas can be derived by complete induction w.r.t. n, using the fundamental commutator (13) as starting point with $n = 1$. Note that the derivatives after the second equal sign in each formula are with respect to operators, not c-numbers. Clearly, we can use (14) to calculate the commutator of $\hat{p}_j$ with *any* function of $\hat{x}_k$ (that is expandable in a Taylor series) and the commutator of $\hat{x}_k$ with *any* function of $\hat{p}_j$. This gives

$$\begin{aligned}[\hat{p}_j, f(\hat{\boldsymbol{x}})] &= \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial \hat{x}_j}f(\hat{\boldsymbol{x}})\,, \\ [\hat{x}_k, g(\hat{\boldsymbol{p}})] &= -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial \hat{p}_k}g(\hat{\boldsymbol{p}})\,. \end{aligned} \tag{15}$$

Note that these are operator relations, they are *not* classical formulas. But now we are in a position to evaluate the Heisenberg equations of motion for our particle, given the Hamiltonian

$$H = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}})\,, \tag{16}$$

and there is no difference between H and H_S, as long as we have energy conservation and H is, therefore, time independent. We have

$$\begin{aligned}\dot{\hat{\boldsymbol{x}}}(t) &= \frac{\mathrm{i}}{\hbar}[H, \hat{\boldsymbol{x}}] = \frac{\mathrm{i}}{\hbar}\left[\frac{\hat{\boldsymbol{p}}^2}{2m}, \hat{\boldsymbol{x}}\right] = -\frac{\mathrm{i}}{\hbar}\left[\hat{\boldsymbol{x}}, \frac{\hat{\boldsymbol{p}}^2}{2m}\right] = -\frac{\mathrm{i}}{\hbar}\left(-\frac{\hbar}{\mathrm{i}}\nabla_{\hat{\boldsymbol{p}}}\frac{\hat{\boldsymbol{p}}^2}{2m}\right) = \frac{\hat{\boldsymbol{p}}(t)}{m}\,, \\ \dot{\hat{\boldsymbol{p}}}(t) &= \frac{\mathrm{i}}{\hbar}[H, \hat{\boldsymbol{p}}] = -\frac{\mathrm{i}}{\hbar}\,[\hat{\boldsymbol{p}}, V(\hat{\boldsymbol{x}})] = -\frac{\mathrm{i}}{\hbar}\left(\frac{\hbar}{\mathrm{i}}\nabla_{\hat{\boldsymbol{x}}}V(\hat{\boldsymbol{x}})\right) = -\hat{\nabla}V(\hat{\boldsymbol{x}})\,, \end{aligned} \tag{17}$$

where I have introduced operator gradients $\nabla_{\hat{\boldsymbol{p}}}$ and $\nabla_{\hat{\boldsymbol{x}}}$ in momentum and position space and renamed the latter to $\hat{\nabla}$. The first of equations (17) demonstrates that the velocity operator $\dot{\hat{\boldsymbol{x}}}$ is equal to the momentum operator divided by m, in nonrelativistic quantum mechanics.[9]

[8] Time derivative operators can be easily constructed in the Schrödinger picture as well. Of course, they are not obtained by taking the time derivative of an operator, which would normally give zero. Rather, we may use the results from the Heisenberg picture and transform back, using $[A(t), B(t)] = \exp(\frac{\mathrm{i}}{\hbar}Ht)[A_S, B_S]\exp(-\frac{\mathrm{i}}{\hbar}Ht)$. Hence, we have $\dot{B}_S = \frac{\mathrm{i}}{\hbar}\,[H, B_S]$ and $\ddot{B}_S = -\frac{1}{\hbar^2}\,[H, [H, B_S]]$. The expectation values of these operators are the first- and second-order time derivatives of the expectation value of B_S, respectively.

[9] This is no longer true in relativistic quantum mechanics as described by the Dirac equation. The relativistic velocity operator has components with discrete eigenvalues $\pm c$, whereas the relativistic momentum operator components still have continuous spectra.

Combining the two equations, we find

$$m\ddot{\hat{\boldsymbol{x}}}(t) = \dot{\hat{\boldsymbol{p}}}(t) = -\hat{\nabla} V(\hat{\boldsymbol{x}})|_{\hat{\boldsymbol{x}}=\hat{\boldsymbol{x}}(t)} \equiv \boldsymbol{F}(\hat{\boldsymbol{x}}(t)) \,, \tag{18}$$

which looks like Newton's equation of motion but of course still is an operator equation. It is fully quantum mechanical and does not describe determinate trajectories. Also, we have not yet taken the limit $\hbar \to 0$. The last equivalence defines the force operator as the negative (operator) gradient of the potential operator.

To approach the topic of trajectories, let us take the expectation value of Eq. (18) with respect to some initial state $|\psi_0\rangle$. We abbreviate $\langle\psi_0|B(t)|\psi_0\rangle = \langle B(t)\rangle$ and obtain

$$m\left\langle \ddot{\hat{\boldsymbol{x}}} \right\rangle = m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{\boldsymbol{x}}\rangle = -\left\langle \hat{\nabla} V(\hat{\boldsymbol{x}}) \right\rangle = \langle \boldsymbol{F}(\hat{\boldsymbol{x}})\rangle \ . \tag{19}$$

This is Ehrenfest's theorem. Here, the left-hand side is the second time derivative of a trajectory, because the expectation value of each component of the vector $\hat{\boldsymbol{x}}$ is a number-valued function of time (and because time derivatives can be commuted with taking the expectation value, in the Heisenberg picture[10]). However, the right-hand side does not quite have the classical form yet: we need a function of the classical trajectory there.[11]

More precisely, what is required to turn Eq. (19) into the classical equation of motion is the relationship

$$\langle \boldsymbol{F}(\hat{\boldsymbol{x}})\rangle = \boldsymbol{F}\left(\langle\hat{\boldsymbol{x}}\rangle\right) \,, \tag{20}$$

because if this is true, we can identify $\boldsymbol{x} = \langle\hat{\boldsymbol{x}}\rangle$ as the classical position vector of the particle and this satisfies

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\boldsymbol{x} = \boldsymbol{F}(\boldsymbol{x}) \,, \tag{21}$$

which is just Newton's second axiom of classical mechanics.

Interestingly, it is trivial to achieve this at time zero. We just have to take an eigenstate of the position operator as the initial state, then the expectation value $\langle \boldsymbol{F}(\hat{\boldsymbol{x}})\rangle$ is equal to $\boldsymbol{F}(\boldsymbol{x})$, where $\boldsymbol{x}$ is the vector of eigenvalues of the components of the position operator in the eigenstate considered, and we obviously have $\langle\hat{\boldsymbol{x}}\rangle = \boldsymbol{x}$. However, this cannot be the full answer, because we have nowhere used that we take the limit $\hbar \to 0$ so far. We need Eq. (20) to hold at all times, not just at the initial time.

I have given the standard hand-waving argument before, why this should be the case: as $\hbar \to 0$, the de Broglie wavelength becomes small and standard deviations of the averages of observables become negligible compared with the expectation values themselves. Then we have $\langle AB\rangle = \langle A\rangle\langle B\rangle$ for any pair of observables A and B and hence Eq. (20) holds.

[10] This is not true in the Schrödinger picture, because the wave function is time-dependent there. In the Schrödinger picture, time dependences of expectation values derive from the time dependence of the wave function, whereas in the Heisenberg picture, they derive from time dependences of the operators. However, in the Schrödinger picture the operator $\ddot{\hat{\boldsymbol{x}}}_S$ is defined as discussed in footnote 8, and then Eq. (19) remains correct with Schrödinger picture operators and expectation values.

[11] For the harmonic oscillator, where $\langle \boldsymbol{F}(\hat{\boldsymbol{x}})\rangle = m\omega^2\langle\hat{\boldsymbol{x}}\rangle$, the form of the equation already corresponds to that of the classical limit, because the gradient of the potential is a linear function of $\hat{\boldsymbol{x}}$ and, hence, Eq. (20) is satisfied automatically.

Here, I would like to be a bit more precise. First, we note, as before, that $\hbar \to 0$ implies that Heisenberg's uncertainty relation does not impose any constraints on the variances of position and momentum components, so we can specify both the initial position and momentum sharply.[12] In particular, the position probability distribution must be a δ function. Second, we must show that under the time evolution of the system, the variance stays zero, meaning that the distribution remains a δ function. This can be done in the Heisenberg picture, but I will take a shortcut here, using a result from the previous subsection. We have, for the expectation value of an arbitrary operator that is a function of $\hat{\boldsymbol{x}}$ only

$$\begin{aligned}\langle B(\hat{\boldsymbol{x}}(t))\rangle &= \langle\psi_0|B(\hat{\boldsymbol{x}}(t))|\psi_0\rangle = \langle\psi(t)|B(\hat{\boldsymbol{x}}_S)|\psi(t)\rangle = \int \mathrm{d}^3x'\psi^*(\boldsymbol{x'},t)B(\boldsymbol{x'})\psi(\boldsymbol{x'},t)\\ &= \int \mathrm{d}^3x' B(\boldsymbol{x'})w(\boldsymbol{x'},t) \end{aligned} \tag{22}$$

and we have shown, using Eq. (9), that $w(\boldsymbol{x'},t) = \delta\left(\boldsymbol{x}(t) - \boldsymbol{x'}\right)$ in the limit $\hbar \to 0$ (if $w(\boldsymbol{x'},0)$ is a δ function). But then we can do the integral in Eq. (22) and obtain $\langle B(\hat{\boldsymbol{x}}(t))\rangle = B(\boldsymbol{x}(t))$. Using this general result with the definitions $B(\hat{\boldsymbol{x}}(t)) = \hat{\boldsymbol{x}}(t)$ and $B(\hat{\boldsymbol{x}}(t)) = \boldsymbol{F}(\hat{\boldsymbol{x}}(t))$, we have $\langle\hat{\boldsymbol{x}}(t)\rangle = \boldsymbol{x}(t)$ and $\langle\boldsymbol{F}(\hat{\boldsymbol{x}}(t))\rangle = \boldsymbol{F}(\boldsymbol{x}(t))$, hence we finally obtain Eqs. (20) and (21). This completes the proof for the Heisenberg picture.

Feynman's path integrals

The central quantity in Feynman's approach to quantum mechanics [2] is the propagator

$$\begin{aligned}Z(\boldsymbol{x}_B,t_2,\boldsymbol{x}_A,t_1) &= \mathcal{N}\int \mathcal{D}x\ \exp\left(\frac{\mathrm{i}}{\hbar}S\big([\boldsymbol{x}(t)]\big)\right)\\ &= \mathcal{N}\int \mathcal{D}x\ \exp\left(\frac{\mathrm{i}}{\hbar}\int_{t_1}^{t_2} L(\dot{\boldsymbol{x}}(t),\boldsymbol{x}(t),t)\,\mathrm{d}t\right)\ , \end{aligned} \tag{23}$$

describing the probability amplitude of a particle starting from point $\boldsymbol{x}_A$ at time t_1 to arrive at point $\boldsymbol{x}_B$ at time t_2. $S\big([\boldsymbol{x}(t)]\big)$ is the classical action of the particle doing so, therefore it is a functional of the path, $\mathcal{N}$ is a normalization factor and the symbol $\mathcal{D}x$ denotes functional integration over all paths going from $(\boldsymbol{x}_A,t_1)$ to $(\boldsymbol{x}_B,t_2)$, so we must have $\boldsymbol{x}(t_1) = \boldsymbol{x}_A$ and $\boldsymbol{x}(t_2) = \boldsymbol{x}_B$. The second equality holds only when the classical action derives from a Lagrangian, which is denoted by L here. In his thesis [2], Feynman gives an example for a system, where the action does not follow from a Lagrangian. "Probability amplitude" has the usual meaning here, i.e., $|Z(\boldsymbol{x}_B,t_2,\boldsymbol{x}_A,t_1)|^2$ is proportional to the probability density of the particle going from $(\boldsymbol{x}_A,t_1)$ to $(\boldsymbol{x}_B,t_2)$.

Now, whenever a classical system is describable by a Lagrangian, we can obtain a Hamiltonian for it (via a Legendre transformation). Quantization of this classical Hamiltonian then allows to write down a Schrödinger equation for the system. The wave function that is solution to the Schrödinger equation may be obtained from Feynman's propagator via multiplication with an initial wave function and integration over all possible initial positions of the particle(s):

$$\psi(\boldsymbol{x},t) = \int \mathrm{d}^3x' Z(\boldsymbol{x},t,\boldsymbol{x'},t_0)\psi(\boldsymbol{x'},t_0)$$

[12] For our second-order equation of motion to have a unique solution, we have to fix an initial value of position and its time derivative, i.e., (up to a factor) momentum.

$$= \mathcal{N} \int \mathrm{d}^3x' \int \mathcal{D}x \, \exp\left(\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} L(\dot{\boldsymbol{x}}(t'), \boldsymbol{x}(t'), t')\,\mathrm{d}t'\right) \, \psi(\boldsymbol{x'}, t_0)$$
$$= \mathcal{N} \int \mathcal{D}'x \, \exp\left(\frac{\mathrm{i}}{\hbar} S\big([\boldsymbol{x}(t')]\big)\right) \, \psi(\boldsymbol{x'}, t_0)\,, \tag{24}$$

where the prime on the differential in the last line is to remind us that now the path integral is not between two fixed points of space-time but that the initial spatial position of the paths is arbitrary, whereas the final one is fixed (as are both the initial and final times). Feynman suggests his approach to be more generally applicable than the Schrödinger equation, as there are classical systems described by an action that does not arise from a Lagrangian, so no classical Hamiltonian description is available that could be quantized à la Schrödinger, whereas the system can be quantized à la Feynman, as long as an action principle is applicable. I will not enter the discussion whether there might be quantum systems for which a Schrödinger equation can be given but no path ingegral. Let me just point out that a minimum requirement for such a system would be that it does not have a classical Hamiltonian (i.e., it must have a quantum Hamiltonian without classical analogue), so no classical Lagrangian can be constructed, and there may be no handle to apply the principle of least action.

Anyway, it was argued that the Feynman picture is just an alternative formulation of the Schrödinger picture, and the argument was probably based on the representation (24) of the wave function or something similar. Now, the wave function is simply the position space representation of a Hilbert vector: $\psi(\boldsymbol{x}, t) = \langle \boldsymbol{x} | \psi(t) \rangle$, and a similar representation in terms of path integrals can be given for position space integral kernels describing operators (i.e., the matrix elements $A(\boldsymbol{x}, \boldsymbol{x'}) = \langle \boldsymbol{x}|A|\boldsymbol{x'}\rangle$). Writing

$$A(\boldsymbol{x}, t, \boldsymbol{x'}, t_0) = \big\langle \boldsymbol{x}\big| A(t-t_0)\big|\boldsymbol{x'}\big\rangle = \left\langle \boldsymbol{x}\right| \exp\left(\frac{\mathrm{i}}{\hbar}H(t-t_0)\right) A_S \exp\left(-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right) \left|\boldsymbol{x'}\right\rangle$$
$$= \int \mathrm{d}^3y \int \mathrm{d}^3y' \left\langle \boldsymbol{x}\right| \exp\left(\frac{\mathrm{i}}{\hbar}H(t-t_0)\right) \left|\boldsymbol{y}\right\rangle \langle \boldsymbol{y}|A_S|\boldsymbol{y'}\rangle \left\langle \boldsymbol{y'}\right| \exp\left(-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right) \left|\boldsymbol{x'}\right\rangle$$
$$= \mathcal{N}_1\mathcal{N}_2 \int \mathcal{D}'x_1 \int \mathcal{D}'x_2 \, \exp\left(-\frac{\mathrm{i}}{\hbar} S\big([\boldsymbol{x_1}(t')]\big)\right) A(\boldsymbol{y}, t_0, \boldsymbol{y'}, t_0) \, \exp\left(\frac{\mathrm{i}}{\hbar} S\big([\boldsymbol{x_2}(t')]\big)\right)\,, \tag{25}$$

where we have used that $\left\langle \boldsymbol{x}\right| \exp\left(-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right) \left|\boldsymbol{x'}\right\rangle$ is precisely the Feynman propagator $Z(\boldsymbol{x}, t, \boldsymbol{x'}, t_0)$, we might argue in the same vein that the Feynman path integral approach is just an alternative formulation of the Heisenberg picture, since we have a direct representation of matrix elements and their time evolution in terms of Feynman path integrals. It then appears that the relationship between the Feynman approach and the Schrödinger picture is not closer than that between the Feynman approach and the Heisenberg picture.[13]

How do we get from Eq. (23) to the classical limit? As $\hbar \to 0$, the imaginary exponent $\mathrm{i}S/\hbar$ grows indefinitely. Oscillatory integrals of this kind can be analytically evaluated by the method of stationary phase. The rationale behind this technique of asymptotic analysis is that with a wildly oscillating integrand, contributions from neighboring pieces of the "integration interval" tend to cancel each other out, except in the vicinity of points, where the exponent does not vary strongly. There we rather have constructive interference. Hence, in the limit, where the large parameter (here $1/\hbar$) grows beyond all bounds, the integral will be dominated by points of stationary phase. What does that mean in the present case? The domain of integration is all paths between two points, so stationarity at a given path means that S does

[13] Arguably, this was at least Feynman's own view.

not change on variation of the paths about this given one. In variational calculus this may be expressed as $\delta S = 0$, and if S results from a Lagrangian, we know how to evaluate the stationary point(s). The stationary point of

$$S = \int_{t_1}^{t_2} L(\dot{\boldsymbol{x}}(t), \boldsymbol{x}(t), t)\, \mathrm{d}t \tag{26}$$

is calculable from the Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}_k} - \frac{\partial L}{\partial x_k} = 0\,, \qquad k = 1, \ldots 3\,. \tag{27}$$

But these are the classical Lagrangian equations of motion for the particle. They yield the classical path that starts at the fixed initial point $(\boldsymbol{x}(t_1), t_1) = (\boldsymbol{x}_A, t_1)$ and ends at $(\boldsymbol{x}(t_2), t_2) = (\boldsymbol{x}_B, t_2)$ minimizing the action between these two points or at least making it stationary. From the method of stationary phase, we gather that in the limit $\hbar \to 0$ the path integral is dominated by a single path,[14] and this turns out to be the classical one. Hence, within Feynman's approach, the limit $\hbar \to 0$ leads to classical mechanics in a very natural way. Once we have solved (27) to obtain the classical trajectory, we do not care about a full evaluation of the path integral anymore, similar to forgetting about the wave function in the Schrödinger picture, once we have the Hamilton-Jacobi equation for the trajectory.

Note that in the Feynman approach, we need not invoke the possibility of choosing sharp initial conditions for $\boldsymbol{x}$ and $\boldsymbol{p}$ as a consequence of the limit, because only the initial position enters the problem. The second boundary condition does not refer to momentum or velocity but to the arrival point, i.e., another condition on $\boldsymbol{x}(t)$.

Conclusions

In this presentation, I have demonstrated two points, first, that quantum mechanics is applicable to macroscopic systems, and second, that it reduces to classical mechanics in the limit $\hbar \to 0$ (for certain Hamiltonian systems).

My demonstration of the first point was not of mathematical nature. Rather, I have pointed out that quantum mechanics has been consistently applied to macroscopic systems essentially from the point of its inception (or even before: Bose condensation was predicted in 1924). In the almost hundred years that have passed since, quantum statistical mechanics, which by definition is the application of quantum mechanics to macroscopic systems, has become a mature field and we know how to describe a multitude of many-particle systems quantum mechanically. The idea that quantum mechanics be not applicable to macroscopic systems can only arise by a narrow-minded focus on certain aspects of quantum mechanics, such as the description by a wave function. But quantum mechanics is much more than this and there may even be quantum mechanical systems that cannot be described by the device wave function. However, quantum mechanics has additional tools that may remain applicable.

Regarding the second point, it turns out that taking the limit $\hbar \to 0$ leads to three different formulations of classical mechanics in the three different representations of quantum mechanics. This is beautiful. The simplest formulation, viz. Newton's law, appears from the Heisenberg

[14] Providing the path integral has the convergence properties that make it a viable description, a point that is difficult and was not solved by Feynman.

picture, and here the derivation is also simplest, if some handwaving is accepted. If mathematical rigor is required, the Heisenberg picture is actually more complicated than the Schrödinger picture, for which I have basically given the rigorous derivation without major gaps. But the approach to classical mechanics from the Schrödinger picture is via the Hamilton-Jacobi equation that may not be particularly familiar to everyone. Nevertheless, it is a standard formulation within Hamiltonian mechanics and part of the regular mechanics courses, so it is not inaccessible at all. Just a bit theoretical. The transition to classical mechanics via the limit $\hbar \to 0$ is very simple and accessible in the Feynman approach, leading to the well-known Lagrangian formulation of classical mechanics. However, here I have skipped all major mathematical difficulties having to do with the convergence properties of the path integrals and the applicability of the method of stationary phase. Clearly, there can be no doubt about the workability of the derivation and the correctness of the result. Notwithstanding, to achieve mathematical rigor here seems difficult. But then my purpose was not mathematical rigor. Rather I wanted to provide enough information so everyone can have a look at the details of the approach they like most and convince themselves of the fact that classical mechanics may be regarded as a subbranch of quantum mechanics.

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