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Methodological Notes

HOW QUANTUM MECHANICS HELPS US UNDERSTAND CLASSICAL MECHANICS

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THE paradoxical title of this note has not resulted from a typesetter's error. Classical mechanics is, of course, simpler than quantum mechanics as a whole, and we have become accustomed to value the intuitive classical explanations of quantum mechanical theories. There are well-known general theorems asserting the profound similarity between the motion of a quantum mechanical wave packet and the classical motion of a particle.

Classical mechanics sometimes enables us to understand even the quite special properties of quantum systems. (The following two examples do not pertain directly to the subject of this note and may be omitted by the reader.) Closed orbits in a classical theory are necessarily reflected in the properties of the corresponding quantum system. Every trajectory is describable by a superposition of wave functions that changes with time. A closed orbit, which is repeated indefinitely without change, can occur only when determinate relations exist between the energies associated with the different wave functions. In quantum mechanics there are two cases of central fields in which the energy levels corresponding to different orbital momenta are exactly degenerate. The first case is the Coulomb potential, where for any given value of n the levels with $0 \leq l \leq n-1$ are degenerate. The second case is the potential of a harmonic oscillator, where degenerate levels have the energy

$$E = \left(n + \frac{3}{2} \right) \hbar\omega$$

with identical parity and orbital momenta $l = n$, $l = n - 2$, $l = n - 4, \ldots l = 1$ or $l = 0$. This quantum mechanical property is associated with the fact that in a Coulomb field and in the field of an harmonic oscillator classical mechanics derives closed trajectories, ellipses having one focus at the Coulomb force center or at the point of oscillatory equilibrium, respectively.

Not only are different magnitudes and directions of the angular momentum (which is normal to the plane of the corresponding orbit) assigned to the different orbits; different directions in the orbital plane (i.e., directions of the semimajor axis) are also assigned. The same properties are possessed by the superposed wave functions with identical energies and different values of l. The degeneracy of these energy levels is entailed by the properties of the classical orbits.

The foregoing examples merely illustrate how classical mechanics helps us to understand quantum laws. But where is the promised nontrivial assistance rendered by quantum mechanics to classical mechanics? A simple example is found in adiabatic invariance. Let us consider the classical oscillator

$$m\ddot{x} = -k^2 x,$$

where the elastic constant k varies slowly with time $[k = k(t)]$. This can be the case of a heavy pendulum bob attached to a suspension of slowly varying length. For any given value of k the frequency is $\omega = k/\sqrt{m}$. In quantum theory the energy assumes the values $n\hbar\omega$, where the states are labeled with the integers n.*

Obviously, a slowly varying system in the n-th quantum state remains in the n-th state; the number n does not change. This is the statement of adiabatic invariance in quantum mechanics, and holds true for $n = 0$ or $n = 1$ in the case of a molecule, or for $n = 10^{30}$ (which is the order of magnitude of n for a clock pendulum). Clearly, for a slow adiabatic change of k, independently of the value of $\hbar$ or the specific value of n, we have

$$E = \text{const} \cdot \omega.$$

The proof of this equation is more complicated in classical mechanics. For any potential that is more complex than $k^2 x^2/2$ we can apply the same considerations, except that the level number n must be obtained differently. We shall confine ourselves to a one-dimensional problem. The stationary wave functions of a one-dimensional finite motion (oscillations) are real. The wave function of the n-th state has n nodes (vanishing points).† This means that n half-waves fit into the region where the oscillations occur.

The de Broglie wavelength of a particle is $2\pi\hbar/p$, where p is the momentum ($p = mv$) and there are $p/2\pi\hbar$ waves per centimeter. During the oscillations the momentum does not remain constant. An integra-

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*When the zero-point energy $\hbar\omega/2$ per degree of freedom is included, the energy of a one-dimensional oscillator becomes $(n + 1/2)\hbar\omega$, and that of a three-dimensional oscillator becomes $(n + 3/2)\hbar\omega$. This correction is not essential for our subsequent discussion.

†We note that this follows necessarily from the condition of orthogonality between the n-th function and all preceding functions — the (n−1)-st, (n−2)-nd etc. down to the zeroth function of the ground state.

tion is required to compute the number of waves fitting between the two extreme points:

$$n \text{ (waves)} = \frac{1}{2\pi\hbar} \int_{x_1}^{x_2} p \, dx.$$

We require the number of nodes, i.e., the number of half-waves, which is obviously twice as large. It is customary not to merely multiply the integral by the number 2, but rather to write the level number in the form

$$n = \frac{1}{2\pi\hbar} \oint p \, dx,$$

where the integration is taken over a closed cycle. The path goes from x_1 to x_2 and returns from x_2 to x_1, so that the first integral is actually doubled. Thus the classical adiabatic invariant for the case of a slowly varying potential is the quantity $\oint p \, dx$, since $\hbar$ and n are constants.

I am fully aware that all of the foregoing discussion is an enormous distortion of the historical development of physics. Classical adiabatic invariants were known long before the invention of quantum theory. In the "old" quantum theory of Bohr and Sommerfeld (prior to the work of Heisenberg and Schrödinger) classical adiabatic invariants were utilized because their dimensions (momentum × length) were the same as those of the Planck constant. Physicists of the older generation do not approve of my pedagogical scheme.

It cannot be denied, however, that present-day pupils and students know the Planck relation between energy and frequency. They know about the existence of quantum mechanics and about the de Broglie wavelength, but they do not know (at least before reaching the third or fourth year of the physics curriculum) about adiabatic invariants.

Adiabatic invariance is important aside from oscillatory systems. The most important example is the motion of a charged particle in a magnetic field; we shall merely refer here to a clearly written and very graphically presented article by Northrop and Teller [Phys. Rev. 117, 215 (1960)].

We note also, for the benefit of better informed readers, that quantum ideas improve our understanding of the conditions for application and the exact fulfillment of adiabatic invariance. In the case of a harmonic oscillator the influence that causes the time dependence of the elastic constant is symmetric with respect to the coordinate origin (x and − x are interchangeable). The parity of the functions clearly remains unaffected; therefore the level number n can vary only by the integers 2, 4, ... (n → n ± 2 → n ± 4, ...).

It therefore becomes clear that the probability of transitions, thus violating adiabatic invariance (which, as already shown, is equivalent to n = const), depends on the Fourier components of the frequency 2ω in the function k(t), since the system uses specific portions of energy in the transitions n → n ± 2. The accuracy of an invariant therefore depends on the precise form of k(t). Parametric resonance is included here; if the time dependent function k(t) is given by

$$k = k_0 + a \cos (2\omega t),$$

then transitions and energy pumping are especially intense.

However, we must conclude this discussion of the harmonic oscillator, lest this "popular" explanation become more complicated than the standard classical treatment.

The second most important case where quantum mechanics is simpler than classical mechanics and helps us to understand the latter consists in the concepts of phase space and the Liouville theorem, which are the basis of statistical physics. In quantum statistical physics we "simply" (in principle) count the number of individual discrete quantum states: 1, 2, 3 etc. States of equal energy are equally probable; in other cases their probabilities are proportional to $\exp(-E_n/kT)$. In scientific terms, within a bounded space (a potential well) the eigenstates of the Hamiltonian form a denumerable set, unlike the continuum of states considered in classical mechanics and classical statistical physics. This fact is responsible for the fundamental simplicity of quantum statistics as compared with classical statistics. It is therefore useful to introduce quantum concepts in order to achieve a better understanding of classical statistics.

The phase volume V_f of classical statistics is proportional to the number of quantum states:

$$N = \frac{1}{(2\pi\hbar)^3} \int d^3p \, d^3x = \frac{V_f}{(2\pi\hbar)^3} ;$$

this equation pertains to a single particle in three-dimensional space. The proof is derived most simply for a potential well having the form of a parallelepiped with the sides X, Y, and Z. Each level corresponds to a whole number of half-waves, so that the allowed values of the particle momentum are

$$p_x = n_x \frac{\pi\hbar}{X} , \qquad p_y = n_y \frac{\pi\hbar}{Y} , \qquad p_z = n_z \frac{\pi\hbar}{z} ;$$

each level corresponds to a point in momentum space and it is easy, for example, to compute the number of such points for the region

$$E = \frac{p^2}{2m} < E_1;$$

we thus obtain

$$N = \frac{1}{(2\pi\hbar)^3} \frac{4\pi}{3} p_1^3 \, XYZ = \frac{1}{(2\pi\hbar)^3} V_f,$$

where $p_1^2/2m = E$. We have considered that $n_x > 0$, $n_y > 0$, and $n_z > 0$; also, the absolute values of p_x, p_y, and p_z were understood in the foregoing discussion.

The relation between a volume in phase space and the number of states has now been derived. We need only know, in addition, that at large values N is addi-

tive,—that the number of levels in two potential wells when added or even interconnected is $N = N_1 + N_2$. Then, if the relation between N and V_f has been obtained for a rectangular well, any functional dependence $U(r)$ of the potential energy on the coordinate r can be constructed out of many rectangular wells. Consequently the Liouville theorem has the simple intuitive meaning that the number of states occupied by a system is conserved during the motion of its particles.

As a special case of the theorem let us consider a Fermi gas at absolute zero. N particles occupy N different quantum levels;* levels with $E < E_f$ (the Fermi energy) are occupied, while levels with $E > E_f$ are empty. When the system is acted on by any forces the levels can be changed so that those occupied by the particles are no longer the very lowest set. As an example, let all momenta be increased by an identical amount p_0. As previously, the N particles will then occupy a compact group of N levels, The entropy had been and remains equal to zero.

Entropy is actually a measure of disorder. Neither completely filled nor empty levels contribute to the

entropy. Contributions to the entropy come only from levels that may or may not be occupied by particles, in each case with a probability p such that $0 < p < 1$. It is not important in calculating the entropy to know whether the very lowest energy levels are occupied. Only the kind of distribution is important, that is, the existence of either a sharp extreme distribution (represented by a region with $p = 1$ and another region where $p = 0$; $S = 0$) or a diffuse distribution. When there exists a region with $0 < p < 1$, then $S = -k\Sigma p \ln p > 0$, where k is the Boltzmann constant.

Classical adiabatic invariance is related to the adiabatic change of quantum levels. Particles then remain on the same levels. This behavior of a quantum system was found to be related, in turn, to the thermodynamic concept of an adiabatic process, in which entropy is conserved.

Quantum concepts thus enable us to couple and to understand better the complex laws of both classical mechanics and classical statistical physics.

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*We here neglect the fact that two particles having spin 1/2 can exist for each spatial level.

Translated by I. Emin