Significance of Ehrenfest theorem in quantum–classical relationship

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The significance of Ehrenfest theorem in quantum–classical relationship is discussed in terms of the general formulation of the theorem. With the ensemble interpretation of the quantum mechanical ψ-function, the Generalized Ehrenfest Theorem reveals some interesting exact relationships between quantum and classical expectation values. These general results seem to imply a deep-rooted unity (in spite of apparent radical differences in conceptual structures) between classical and quantum mechanics. Some significant consequences and important physical insights which follow from the general formulation are discussed with examples. Most important is that it offers, under reasonable approximations, a pure quantum mechanical description of the Stern–Gerlach experiment with realistic inhomogeneous magnetic field (∇.B = 0).

EVEN almost seventy-five years after the first formulation of quantum mechanics (QM), its relation with classical mechanics (CM) remains obscure. The usual belief that QM has superseded CM is also not well founded. In all cases where a new theory supersedes an old one, there is a universal prescription of recovering the mathematical structure of the old theory in the domain of its validity, i.e. where it is empirically established. This is true for both special and general theory of relativity[1]. But for QM, no such universal approximation procedure can be offered. About the success and failure of the two mechanics we can make two positive assertions: (i) There are experimental results in the microscopic domain (such as hydrogen spectrum) or in the macroscopic domain (such as specific heat of solids at low temperature) which cannot be interpreted within the framework of CM. (ii) In all such cases, the mathematical formalism of QM provides the correct empirical results. Not a single failure has yet been reported.

These empirical evidences show that CM cannot be the universal mechanics and that QM has such a potentiality. However, since it is not yet possible to recover CM in all the domains of its validity, we cannot assert that QM has superseded CM. A second alternative that both CM and QM have restricted domains of validity remains open[2]. Also, there are indications that some classical ensembles have properties which may not have any parallel in QM[3].

Many textbooks[4,5] give the impression that Ehrenfest theorem (ET)[6] leads to CM in the limit of macroscopic bodies, represented by localized packets. Ballentine *et al.*[7] have shown that ET is neither sufficient nor necessary for approaching the classical regime. One may then ask, what is the significance of this theorem? This question has rarely been addressed. We show in this paper that ET in its generalized form (see the next section), reveals some interesting exact relations between CM and QM. If we interpret ψ-function to represent an ensemble of particles, then in a class of situations, it can be shown that the expectation values of a group of dynamical variables develop in time exactly the same way as those of a classical ensemble whose time development is governed by Liouville's equation. This identical dynamical behaviour for quantum and classical ensembles, though in restricted situations, indicates some deeper unity between the two mechanics which lies hidden behind their widely different mathematical and conceptual structures.

To regard a ψ-function as describing the properties of an ensemble[8] has one merit that the disturbing question whether the quantum principle of superposition of states remains valid in the classical region is no longer relevant. Besides, the basic observable quantities of QM (distribution functions and expectation values of dynamical variables) can be interpreted for a classical ensemble without difficulty.

Generalized Ehrenfest Theorem

We take the Hamiltonian as:

$$H = \frac{1}{2m}(\mathbf{P} - e\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r}). \tag{1}$$

Then the ET takes the form:

$$\frac{\mathrm{d}\langle r_k \rangle}{\mathrm{d}t} = \frac{1}{m}\langle p_k - eA_k \rangle,$$

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$$\frac{\mathrm{d}\langle p_k - eA_k\rangle}{\mathrm{d}t} = -\left\langle \frac{\partial V}{\partial r_k}\right\rangle + \frac{e}{m}\{\langle(\mathbf{p} - e\mathbf{A})\rangle \times \mathrm{curl}\mathbf{A}\}_k, \qquad (2)$$

where all the expectation values are calculated with respect to $\psi(\mathbf{r}, t)$ which is a solution of the Schrödinger equation. Most discussions on ET are confined to the case $\mathbf{A} = 0$. As the generalization to the Hamiltonian (eq. (1)) is straightforward, we do not include a proof. Equations (2) can be generalized[9] for an arbitrary dynamical variable $f(q_i, p_i)$, where q_is are the generalized configuration coordinates and p_is are the corresponding conjugate momentum coordinates. If we consider a quantum system with the Hamiltonian $H = H(q_i, p_i)$, the time development of the expectation value of $f(q_i, p_i)$ in the state $\psi(q_i, t)$ of the system is given by:

$$\frac{\mathrm{d}\langle f\rangle}{\mathrm{d}t} = \frac{1}{i\hbar}\langle[f, H]\rangle. \qquad (3)$$

For the Hamiltonian (eq. (1)), eq. (2) follows from eq. (3) with the special choices, $f = r_k$ and $(p_k - eA_k)$, respectively.

Corresponding to the quantum ensemble represented by $\psi(q_i, t)$, we imagine a classical ensemble described by a normalized phase space density function $\rho_c(q_i, p_i, t)$. The expectation value (ensemble average) of the dynamical variable f is defined by:

$$\langle f\rangle_c = \int f(q, p)\, \rho_c(q, p, t)\, \mathrm{d}q\mathrm{d}p. \qquad (4)$$

The phase space density function ρ_c satisfies the Liouville equation:

$$\frac{\partial \rho_c}{\partial t} = -\{\rho_c, H\}_{\mathrm{PB}}, \qquad (5)$$

where the right hand side is the classical Poisson bracket. From eqs (4) and (5) we get, after partial integration (using proper boundary conditions for ρ):

$$\frac{\mathrm{d}\langle f\rangle_c}{\mathrm{d}t} = \langle\{f, H\}_{\mathrm{PB}}\rangle. \qquad (6)$$

In the following we argue that the similarity between eqs (3) and (6) is more than formal. In terms of appropriate expectation values they are exactly equivalent. Both quantum commutations and classical Poisson brackets satisfy the same rule of decomposition:

$$[f, p_i p_j] = p_i[f, p_j] + [f, p_i]p_j,$$

and,

$$[q_i, p_j]/(i\hbar) = \delta_{ij} = \{q_i, p_j\}_{\mathrm{PB}}. \qquad (7)$$

In general, f is of the form:

$$f = \Sigma_m f_m,\ f_m = R_m(\mathbf{r}) p_1^{m_1} p_2^{m_2} p_3^{m_3} + p_1^{m_1} p_2^{m_2} p_3^{m_3} R_m(\mathbf{r}),$$

where R_m is an arbitrary function of $\mathbf{r}$. Obviously, f_m and f are Hermitian operators in QM. When the brackets are decomposed, the right hand side of both the eqs (3) and (6) will contain the same set of expectation values. However, the right hand side of eq. (6) on simplification shows that, in the classical case the Hermitian ordering of the variables is absent. For example, a term like $qp + pq$ in eq. (3) will appear as $2qp$ in eq. (6) – the ordering has no significance in CM. On the other hand, after the commutators are decomposed, the right hand side of eq. (3) will not contain $\hbar$ explicitly and the two expressions (eqs (3) and (6)) are exactly equivalent. This is a rather surprising result as no physical reason seems to demand such an exact similarity. Ballentine *et al.*[7] have derived the result for a scalar potential field only for the time derivative of momentum expectation value. By repeated application of eq. (3), we get a system of linear equations, which may or may not be closed with respect to the number of independent expectation values. In the former case, say, n different expectation values give n first-order equations. If a classical phase space density at $t = 0$ is so chosen that initially all the n expectation values are the same as in the quantum ensemble, then their time development will be identical. We can then replace quantum calculations by classical ones. This important conclusion follows from the generalization of ET, developed here in terms of Liouville's theorem. It may appear that in cases where classical and quantum mechanical expectation values develop in time in an identical manner (e.g. when the Generalized Ehrenfest Theorem (GET) leads to a finite coupled set of expectation value evolution equations), Wigner phase space density formulation of QM provides a clue to this surprising result. This, however, is not true. If we take $f(q, p)$ in the form:

$$f(q, p) = g(q) + h(p),$$

Wigner phase space density determined from the quantum mechanical ψ function yields correct quantum expectation value of f at all times[10]. But Wigner phase space density function satisfies the Liouville's equation only approximately and it is well known that it is not always positive definite.

ET is usually expressed in terms of eq. (2). Some workers like Ballentine *et al.*[7] have designated ET by an approximate expression, replacing $\langle V(\mathbf{r})\rangle$ by $V(\langle\mathbf{r}\rangle)$ in eq. (2) – forming a closed set of equations in $\langle\mathbf{r}\rangle$ and $\langle(\mathbf{p} - e\mathbf{A})\rangle$ which are seldom exact. In a recent paper, Ballentine and McRae[11] have thoroughly investigated the 'corrections to ET' in terms of the moment equa-

tions for probability distributions for both regular and chaotic motions. They have shown that for sufficiently narrow probability distributions, a truncation of the 'moment hierarchy' provides a useful method for comparing quantum and classical evolutions and for studying differences between regular and chaotic motions.

However, their main emphasis is on the problem of classical limit and the emergence of classical behaviour from QM. One most significant aspect of ET of some operational importance remains unexplored. With the general expression for the ET (eq. (3)), we get a number of closed sets of equations which are exact. In some other cases, closed sets of equations may be obtained under well-defined approximations. There are some significant consequences which follow from the GET. A beam of charged particles of constant energy when subjected to a uniform electric or magnetic field will suffer a mean deflection which will be identical in CM and QM. If the beam is narrow, then it would appear that the particles are following a classical track. This result is independent of the energy and the width of the beam. It also explains why in all early experiments on electrons, protons, etc. CM has been successfully used and even in precise experiments as in mass spectrometers or β-ray spectrometers, no deviation from classical laws was detected. Classical equations of motion are also used in nuclear induction method for the measurement of magnetic moments of nucleons (see the section on precession of the polarization vector). On the other hand, the general form of eq. (3) allows an extension beyond the usual phase space variables to others. A particle with spin is inconceivable in CM. However, as mathematical objects, spinors are not special to QM, their use in classical rigid dynamics is rather well known. The rotations described by the spinor components have corresponding representations in terms of Eulerian angles[2]. Moreover, without seeking a classical analogue, in some cases the system of equations may be solved directly. We have briefly discussed that approximate solution of the set of equations follows from GET in realistic Stern–Gerlach magnetic field. In the section on Virial theorem and GET, quantum virial theorem is derived from GET and some interesting consequences are discussed. We, therefore, think that *the importance of GET by far transcends its 'inadequacy to characterize the classical regime'*.

We would like to mention a restrictive condition about the closure of the system of equations for expectation values. In all the examples discussed in the following sections, exact set of closed relations are obtained in cases where the potential is at most quadratic. Trials with different potentials indicate that, beyond quadratic potential, perhaps it is not possible to obtain a closed set of first-order differential equations (in time) for expectation values. But, no formal proof of this impossibility seems to exist. Also it appears that there is ample scope of application of this method for systems giving closed set under reasonable approximations. Moreover, it will be shown elsewhere that the closed set of equations can be obtained with higher-order time derivatives of expectation values even for potentials beyond quadratic form.

Closed relations from GET

Deflection of a charged particle in uniform electric and magnetic field

The Hamiltonian for this case is:

$$H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}(\mathbf{r}))^2 - eE_0\hat{k}.\mathbf{r}. \tag{8}$$

Both the electric field $E_0\hat{k}$ and magnetic field $B_0\hat{k}$ are along the z-direction, where $\mathbf{A} = B_0(-y, x, 0)/2$. Application of eq. (3) gives us the following system of first-order equations:

$$\frac{\mathrm{d}\langle\mathbf{r}\rangle}{\mathrm{d}t} = \frac{1}{m}\langle\mathbf{p} - e\mathbf{A}\rangle,$$

$$\frac{\mathrm{d}\langle\mathbf{p} - e\mathbf{A}\rangle}{\mathrm{d}t} = eE_0\hat{k} + \frac{e}{m}\langle(\mathbf{p} - e\mathbf{A})\rangle \times \mathrm{curl}\mathbf{A}. \tag{9}$$

These two equations form a closed set for the expectation values $\langle\mathbf{r}\rangle$ and $\langle(\mathbf{p}–e\mathbf{A})\rangle$. Thus the mean deflection for a quantum ensemble will be exactly the same as that of a classical ensemble. If the beam of particles is narrow, then one can calculate the deflection from the classical track of a single particle. This is the real justification why in highly precise instruments like mass spectrometer, β-ray spectrometer deflections are always calculated by using classical laws and no quantum correction is necessary. By adding four more equations to the above two we get another closed set involving six expectation values. These four equations are:

$$\frac{\mathrm{d}\langle\mathrm{r}^2\rangle}{\mathrm{d}t} = \frac{1}{m}\langle\mathbf{r}.\mathbf{p} + \mathbf{p}.\mathbf{r}\rangle,$$

$$\frac{\mathrm{d}\langle\mathbf{r}.\mathbf{p} + \mathbf{p}.\mathbf{r}\rangle}{\mathrm{d}t} = \frac{2}{m}\langle p^2\rangle - \frac{e}{m}\langle\mathbf{p}.\mathbf{A} + \mathbf{A}.\mathbf{p}\rangle + 2eE_0\hat{k}.\langle\mathbf{r}\rangle,$$

$$\frac{\mathrm{d}\langle\mathbf{p}.\mathbf{A} + \mathbf{A}.\mathbf{p}\rangle}{\mathrm{d}t} = 0,$$

$$\frac{\mathrm{d}\langle p^2\rangle}{\mathrm{d}t} = 2eE_0\hat{k}.\langle\mathbf{p}\rangle. \tag{10}$$

Thus dispersion in position and momentum for the ensemble can also be calculated classically without making any error.

Dispersion in a harmonic oscillator potential

For a linear harmonic oscillator the Hamiltonian is:

$$H = p^2/(2m) + m\omega^2 x^2/2. \tag{11}$$

We can get the well-known closed set for $\langle x\rangle$ and $\langle p\rangle$ showing that these average values execute classical motions. But we can get another closed set involving dispersions. These equations are:

$$\frac{d\langle x^2\rangle}{dt} = \frac{1}{m}\langle xp + px\rangle,$$

$$\frac{d\langle xp + px\rangle}{dt} = \frac{2}{m}\langle p^2\rangle - 2m\omega^2\langle x^2\rangle,$$

$$\frac{d\langle p^2\rangle}{dt} = -m\omega^2\langle xp + px\rangle. \tag{12}$$

This set of equations can be solved with suitable initial conditions. Let us take the initial state vector to be a Gaussian function such that $\langle x\rangle = \langle p\rangle = 0$. For such a function $\langle xp + px\rangle$ is also zero. From eq. (12) we get the following second-order differential equations for $\langle x^2\rangle$ and $\langle p^2\rangle$:

$$\frac{d^2\langle x^2\rangle}{dt^2} = 2(\langle p^2\rangle/m^2 - \omega^2\langle x^2\rangle),$$

$$\frac{d^2\langle p^2\rangle}{dt^2} = -2\omega^2\langle p^2\rangle + 2m^2\omega^4\langle x^2\rangle. \tag{13}$$

The initial conditions are, at $t = 0$:

$$\langle x^2\rangle = \sigma_x^2(0); \langle p^2\rangle = \sigma_p^2(0); \frac{d\langle x^2\rangle}{dt} = \frac{d\langle p^2\rangle}{dt} = 0.$$

The solution can be easily found by noting that eq. (12) leads to the result, $m^2\langle x^2\rangle + \langle p^2\rangle/\omega^2$ = a constant, independent of time. The solutions are:

$$m^2\langle x^2\rangle = \frac{1}{2}(m^2\sigma_x^2(0) + (\sigma_p^2(0)/\omega^2)) + \frac{1}{2}(m^2\sigma_x^2(0) - (\sigma_p^2(0)/\omega^2))\cos 2\omega t,$$

and

$$\langle p^2\rangle/\omega^2 = \frac{1}{2}(m^2\sigma_x^2(0) + (\sigma_p^2(0)/\omega^2)) - \frac{1}{2}(m^2\sigma_x^2(0) - (\sigma_p^2(0)/\omega^2))\cos 2\omega t. \tag{14}$$

It is enormously difficult[12] to get these results by solving Schrödinger equation. Correspondingly we can start with a classical phase space density function as:

$$\rho(x, p) = |\psi(x)|^2\,|\phi(p)|^2, \tag{15}$$

where $\psi(x)$ is the Gaussian function assumed above and $\phi(p)$ its Fourier transform. The time development of dispersion in position and momentum of course remains the same as in eq. (14).

Precession of the polarization vector

The Hamiltonian of a spinning charged particle in a magnetic field **B** is:

$$H = -\gamma\,\mathbf{S}.\mathbf{B},$$

where **S** is the spin angular momentum; the proportionality constant γ is the gyromagnetic ratio. Using the properties of Pauli spinors, one can readily obtain from eq. (3):

$$\frac{d\langle\mathbf{S}\rangle}{dt} = \gamma\langle\mathbf{S}\rangle \times \mathbf{B}.$$

A classical analogue of this equation is possible and is discussed by Holland[2]. With the Eulerian representation of the Pauli spinors, the precessional equation of motion of the spin vector in a magnetic field is given by:

$$\frac{d\mathbf{S}}{dt} = \gamma\,\mathbf{S} \times \mathbf{B},$$

which becomes identical with the quantum result in terms of appropriate averages for various orientations of the spin in the ensemble. This can also be expressed in terms of a canonical Poisson bracket relation.

Now if we take $\mathbf{B} = B_0\hat{k}$, then we get

$$\frac{d\langle S_x\rangle}{dt} = \omega\langle S_y\rangle, \frac{d\langle S_y\rangle}{dt} = -\omega\langle S_x\rangle,$$

$$\frac{d\langle S_z\rangle}{dt} = 0, \tag{16}$$

where $\omega = \gamma B_0$ is the Larmor frequency. Also from eq. (16) we get the following closed set of equations of motion for $\langle S_x\rangle$ and $\langle S_y\rangle$:

$$\frac{d^2\langle S_x\rangle}{dt^2} = -\omega^2\langle S_x\rangle; \frac{d^2\langle S_y\rangle}{dt^2} = -\omega^2\langle S_y\rangle.$$

Thus the time dependence of expectation values follows exactly the classical equation of motion for angular momentum vector. In the measurement of magnetic moment of neutron and other nuclei by the nuclear induction method, Bloch[13] has used essentially these classical equations dispensing with the Schrödinger equation from the simple argument based on ET.

Stern–Gerlach experiment

Pure quantum mechanical description of the process using realistic inhomogeneous magnetic field is lacking in the literature. For a realistic Stern–Gerlach field ($\nabla.\mathbf{B} = 0$), the Hamiltonian may be written as:

$$H = p^2/(2m) - \gamma\, \mathbf{S}.\mathbf{B},$$

where $\mathbf{B}$ is taken as:

$$\mathbf{B} = B_0\hat{k} - \mathbf{B_1}; \mathbf{B}_1 = b(-x,0,z).$$

Using eq. (3) we have the following equations:

$$\frac{d\langle\mathbf{S}\rangle}{dt} = \gamma B_0\langle\mathbf{S}\rangle\times\hat{k} - \gamma\langle\mathbf{S}\times\mathbf{B}_1\rangle,$$

and

$$\frac{d^2\langle\mathbf{r}\rangle}{dt^2} = \frac{\gamma}{m}\langle\nabla(\mathbf{S}.\mathbf{B}_1)\rangle. \quad (17)$$

In general eq. (17) do not form a closed set. But if we assume that the dynamics of $\langle\mathbf{S}\rangle$ is mainly determined by $B_0\hat{k}$ and the effect of the inhomogeneous field is weak enough to produce entanglement between space and spin states of the silver atoms, as a reasonable approximation we may then write, $\langle zS_y\rangle = \langle z\rangle\langle S_y\rangle$, etc. and the eq. (17) forms a closed set. Appropriate initial conditions result in a deflection of the beam of Stern–Gerlach atoms only in the z-direction, given by (Sen and Sengupta, unpublished):

$$\langle z\rangle = \frac{\gamma}{2m} b\langle S_z\rangle t^2,$$

after time t spent within the inhomogeneous field.

Thus GET provides a quantum mechanical description of Stern–Gerlach experiment under reasonable approximations. The usual semiclassical argument[14] based on Larmor precession in replacing realistic inhomogeneous field by idealized field ($\nabla.\mathbf{B} \neq 0$) is inadequate and cannot offer a correct physical insight of the problem.

Virial theorem and GET

If we consider a single particle of mass m moving in a potential field $V(\mathbf{r})$, then from classical equations of motion we arrive at the result:

$$\frac{1}{\tau}[m\dot{\mathbf{r}}.\mathbf{r}]_0^\tau = \langle m\dot{r}^2\rangle_r - \langle\mathbf{r}.\nabla V\rangle_\tau,$$

where the time average is taken over an arbitrary time interval τ. For a bounded system, the left hand side will vanish in the large time limit and we get the usual statement of classical virial theorem:

$$2\langle T\rangle_\tau = \langle\mathbf{r}.\nabla V\rangle_\tau, \quad (18)$$

where T is the kinetic energy of the system. If we have an ensemble of particles, then each particle satisfies eq. (18). Hence if we take the ensemble average over a phase space density function ρ then,

$$2\langle\langle T\rangle_\tau\rangle_\rho = \langle\langle\mathbf{r}.\nabla V\rangle_\tau\rangle_\rho. \quad (19)$$

This is the classical virial theorem for an ensemble. The ordering of the two averages can be reversed in the classical theory without affecting the result.

From GET we get for a quantum system with Hamiltonian, $H = T + V(\mathbf{r})$, in an arbitrary state ψ:

$$\frac{d\langle\mathbf{r}.\mathbf{p}\rangle_\psi}{dt} = \frac{1}{i\hbar}\langle[\mathbf{r}.\mathbf{p}, H]\rangle_\psi. \quad (20)$$

Evaluating the commutators we finally get the quantum mechanical virial theorem given by:

$$\frac{d\langle\mathbf{r}.\mathbf{p}\rangle_\psi}{dt} = 2\langle T\rangle_\psi - \langle\mathbf{r}.\nabla V\rangle_\psi.$$

Taking average over sufficiently long time, the left hand side will go to zero for a bounded system and we get the general form of the quantum virial theorem,

$$2\langle\langle T\rangle_\psi\rangle_\tau = \langle\langle\mathbf{r}.\nabla V\rangle_\psi\rangle_\tau. \quad (21)$$

Equation (21) is equivalent to the classical result in eq. (19). This is another example in which we obtain from GET identical relation for classical and quantum expectation values.

For stationary states the left hand side of eq. (20) is identically zero and the quantum virial theorem reduces to:

$$2\langle T\rangle_\psi = \langle \mathbf{r}.\nabla V\rangle_\psi. \quad (22)$$

The physical content of this equation is different from that of the classical eq. (18) for a single particle. However, for a simple power law potential function with the Hamiltonian of the form:

$$H = p^2/(2m) + \alpha q^n,$$

where α is a constant and n is an integer, the expressions for classical and quantum virial theorems are, respectively, given by:

$$\langle T\rangle_\tau = \frac{n}{2}\langle V\rangle_\tau,$$

and

$$\langle T\rangle_\psi = \frac{n}{2}\langle V\rangle_\psi,$$

If the total energy for the classical particle is taken equal to the energy eigenvalue of the corresponding quantum stationary state, then the classical time averages of T and V are exactly equal to the quantum mechanical expectation values, i.e. $\langle T\rangle_\tau = \langle T\rangle_\psi$, etc. Textbook examples of such results are available for linear harmonic oscillator[15] and also for hydrogen atom (ref. 9, p. 228) problems. But it is evident that a similar result follows for any system with single component power law potential function.

Discussion

We believe that the most important significance of GET lies in developing closed set of equations for the mean values of several variables. Repeated application of eq. (3) thus provides equations of motion for the closed set of variables. We can then either solve the system of equations if these are not too complicated or take advantage of the classical analogue to arrive at a solution. In the case of the Stern–Gerlach experiment, reasonable approximation necessary for getting closed set of quantum equations of motion flowing from eq. (3), immediately reproduces results of standard semiclassical calculations of the Stern–Gerlach effect. However, the class of systems for which closed set of equations may be obtained is to be determined by trial and cannot be identified *a priori*.

Another important consequence of GET is the quantum virial theorem. Appropriate virial theorem is of immense importance in both classical physics (kinetic theory of gases) and in quantum theory (lattice mechanical studies[16], nuclear physics[17], etc.). The usual version of quantum virial theorem is not general (applies only to stationary states) and formally different from the classical virial theorem. From GET we have derived the general statement which involves both the time and ensemble averages and the complete formal identity between the classical and quantum virial theorem is established.

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