



Derivation of the Schrödinger Equation from Classical Stochastic Dynamics

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Abstract

From classical stochastic equations of motion, we derive the quantum Schrödinger equation. The derivation is carried out by assuming that the real and imaginary parts of the wave function ϕ are proportional to the coordinates and momenta associated with the degrees of freedom of an underlying classical system. The wave function ϕ is assumed to be a complex time-dependent random variable that obeys a stochastic equation of motion that preserves the norm of ϕ . The quantum Liouville equation is obtained by considering that the stochastic part of the equation of motion changes the phase of ϕ but not its absolute value. The Schrödinger equation follows from the Liouville equation. The wave function ψ obeying the Schrödinger equation is related to the stochastic wave function by $|\psi|^2 = \langle |\phi|^2 \rangle$.

Keywords Schrödinger equation · Quantum Liouville equation · Stochastic dynamics

Schrödinger introduced the quantum wave equation that bears his name [1–7] by using an analogy between mechanics and optics. Hamilton had shown that there is a relation between the principle of least action of mechanics and the geometric optics. Considering that the Hamilton equation [8–11] of motion of classical mechanics is analogous to the equation of geometric optics, there must be a wave equation, the Schrödinger equation, which is the analogous of the light wave equation.

As the theories of motion based on the Hamilton equation and on the Schrödinger equation describe the same phenomena, they are conflicting theories as they predict different results at small scales. However, at large scales, they give the same results, and we may say that in this regime, it is possible to derive the classical Hamilton equation from the Schrödinger equations. The opposite is never true, what seems to be in contradiction with the title of this paper. However, what concerns us here is not the derivation of quantum mechanics from classical mechanics, but the derivation of the abstract framework of the former from that of the latter.

The derivation is accomplished by representing the motion of a quantum particle by the motion of an *underlying* classical system with many degrees of freedom. The

coordinate and momentum associated with each degree of freedom are considered to be proportional to the real and imaginary parts of a dynamic variable ϕ . This relation makes the complex variables ϕ and ϕ^* a pair of canonically conjugate variables of the classical underlying system. In other words, the states of the underlying system are represented by a phase space with complex components.

The variable $\phi(x)$ is considered to depend on a continuous parameter x and is identified as the wave function of the quantum system. An observable is represented by a bilinear functional of $\phi(x)$ and $\phi^*(x)$, considered to be independent variables. This property of the Hamiltonian makes the norm of $\phi(x)$ a constant of the motion. This is an essential property of the underlying system which is equivalent to preservation of the inner product of a quantum state vector. As the inner product is preserved, the complex phase space becomes a Hilbert space, and we may say that the motion of the classical underlying system is represented in a Hilbert space [12, 13].

The probabilistic character of quantum mechanics is introduced considering the wave function ϕ a stochastic variable which means to turn the equation of motion of the underlying system into a stochastic equation of motion. This is obtained by adding a noise to the Hamilton equation of motion of the underlying system which preserves the norm of ϕ so that the full stochastic equation of motion preserves the norm.

The present approach is different from previous attempts to represent to relate quantum mechanics to classical stochastic dynamics [14, 15]. Usually, in these approaches, the

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position of the quantum particles is treated as a stochastic variable. In our approach, the wave function $\phi(x)$ itself is a random variable or more precisely a complex random field variable.

The underlying system that we consider here is a classical continuous system in one dimension, whose Hamilton equations of motion are

$$\frac{\partial q}{\partial t} = \frac{\delta \mathcal{H}}{\delta p}, \quad \frac{\partial p}{\partial t} = -\frac{\delta \mathcal{H}}{\delta q}, \quad (1)$$

where \mathcal{H} is the Hamiltonian, which is a functional of the coordinate $q(x)$ and the canonical momentum $p(x)$, and we are using a δ to denote the functional derivative.

Instead of the pair of real canonical variables (q, p) , we use new variables which are complex variables obtained through the transformation $\phi = \alpha q + i\beta p$ and $\phi^* = \alpha q - i\beta p$, where α and β are real constants such that $\alpha\beta = 1/2\mu$, and μ is some constant. The new pair (ϕ, ϕ^*) constitutes a pair of canonically conjugate variables, in terms of which the equations of motion become

$$i\mu \frac{\partial \phi}{\partial t} = \frac{\delta \mathcal{H}}{\delta \phi^*}, \quad i\mu \frac{\partial \phi^*}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \phi}, \quad (2)$$

where ϕ and ϕ^* are treated as independent variables, and \mathcal{H} is now considered a functional of $\phi(x)$ and $\phi^*(x)$.

Defining the Poisson brackets between two functionals \mathcal{A} and \mathcal{B} of $\phi(x)$ and $\phi^*(x)$ by

$$\{\mathcal{A}, \mathcal{B}\} = \int \left(\frac{\delta \mathcal{A}}{\delta \phi} \frac{\delta \mathcal{B}}{\delta \phi^*} - \frac{\delta \mathcal{B}}{\delta \phi} \frac{\delta \mathcal{A}}{\delta \phi^*} \right) dx, \quad (3)$$

then the Hamilton equations can also be written in terms of Poisson brackets

$$i\mu \frac{\partial \phi}{\partial t} = \{\phi, \mathcal{H}\}, \quad i\mu \frac{\partial \phi^*}{\partial t} = \{\phi^*, \mathcal{H}\}. \quad (4)$$

It is worth pointing out that the canonically conjugate variables q and p are related by $\{q, p\} = i\mu$.

The Hamiltonian \mathcal{H} of the underlying continuous classical system is assumed to be a bilinear functional in $\phi(x)$ and $\phi^*(x)$,

$$\mathcal{H} = \int \phi^*(x) H(x, x') \phi(x') dx dx'. \quad (5)$$

where $H(x, x') = H^*(x', x)$ so that \mathcal{H} is real. The norm of $\phi(x)$, defined by

$$\mathcal{N} = \int \phi^*(x) \phi(x) dx, \quad (6)$$

is also understood as a function of $\phi(x)$ and $\phi^*(x)$. It is easily seen that \mathcal{H} of the form (5) commutes in the Poisson sense with \mathcal{N} ,

$$\{\mathcal{N}, \mathcal{H}\} = 0, \quad (7)$$

which means that the norm is a constant of the motion. We choose this constant to be equal to the unity.

If we insert the functional (5) into the equation of motion, either (2) or (4), we find

$$i\mu \frac{\partial \phi}{\partial t} = \int H(x, x') \phi(x') dx'. \quad (8)$$

From now on, we assume that the wave function ϕ is a stochastic variable, that is, a time-dependent random variable. It obeys a stochastic dynamics [16–19], which we assume to be the equation of motion (8) supplemented by a stochastic term,

$$\frac{\partial \phi(x)}{\partial t} = \frac{1}{i\mu} \int H(x, x') \phi(x') dx' + \zeta(x, t), \quad (9)$$

where $\zeta(x, t)$ is the stochastic variable representing the white noise.

The stochastic variable ζ is chosen so that the trajectory in the vector space spanned by $\phi(x)$ preserves the norm (6). To set up a noise of this type, we proceed as follows. We discretize the time in intervals τ and write the Eq. (9) in the discretized form

$$\delta \phi(x) = \tau f(x) + i\sqrt{\tau} g(x) \xi - \frac{1}{2} \tau k(x), \quad (10)$$

where ξ is a random variable with zero mean and variance equal to the unity, and f , g , and k are functions of x , given by

$$f = \frac{1}{i\mu} \int H(x, x') \phi(x') dx', \quad (11)$$

$$g = \int G(x, x') \phi(x') dx', \quad (12)$$

$$k = \int K(x, x') \phi(x') dx'. \quad (13)$$

The increment in the norm due to an increment in ϕ is

$$\begin{aligned} \delta \mathcal{N} = \tau \int (f \phi^* + \phi f^*) dx + i\sqrt{\tau} \xi \int (g \phi^* - \phi g^*) dx \\ + \frac{1}{2} \tau \int (2g g^* - k \phi^* - \phi k^*) dx. \end{aligned} \quad (14)$$

The first term vanishes identically, and the second term equals

$$i\sqrt{\tau} \xi \int [(G(x', x) - G^*(x, x')) \phi(x) \phi(x')^* dx' dx]. \quad (15)$$

The last term vanishes if we choose K to be related to G by

$$K(x, x') = \int G(y, x') G^*(y, x) dy. \quad (16)$$

If we choose $G(x', x) = G^*(x, x')$ then $\delta\mathcal{N}$ vanishes identically and \mathcal{N} will be invariant along a trajectory in the vector space in spite of the trajectory being stochastic. If this condition is not satisfied, $\delta\mathcal{N}$ will vanish in the average and $\langle\mathcal{N}\rangle$ will be constant which we choose to be equal to unity.

Let us determine the increment in $\phi(x)\phi^*(x')$. Up to terms of order τ , it is given by

$$\begin{aligned} \delta(\phi_1\phi_2^*) &= \tau(f_1\phi_2^* + \phi_1f_2^*) + \sqrt{\tau}\xi(g_1\phi_2^* + \phi_1g_2^*) \\ &\quad + \tau(k_1\phi_2^* + \phi_1k_2^* + g_1g_2^*), \end{aligned} \quad (17)$$

where we are using the indices 1 and 2 to denote functions of x and x' , respectively. Taking the average of this equation, the second term proportional to $\sqrt{\tau}$ vanishes. Dividing the result by τ , we find the equation for the time evolution of the covariances $\rho(x, x') = \langle\phi(x)\phi^*(x')\rangle$,

$$\frac{\partial\rho(x, x')}{\partial t} = \langle f_1\phi_2^* + \phi_1f_2^* \rangle + \frac{1}{2}\langle 2g_1g_2^* - k_1\phi_2^* - \phi_1k_2^* \rangle. \quad (18)$$

Replacing the expressions of f , g , and k in this equation, we find

$$\begin{aligned} \frac{\partial\rho(x, x')}{\partial t} &= \frac{1}{i\mu} \int [H(x, y)\rho(y, x') - \rho(x, y)H(y, x')] dy \\ &\quad + \int G(x, y)\rho(y, y')G^*(x', y') dy dy' \\ &\quad - \frac{1}{2} \int G^*(y', x)G(y', y)\rho(y, x') dy dy' \\ &\quad - \frac{1}{2} \int \rho(x, y)G^*(y', y)G(y', x') dy dy'. \end{aligned} \quad (19)$$

As the norm is preserved in the average, it follows from (6) that

$$\int \rho(x, x) dx = 1. \quad (20)$$

The Eq. (19) is a closed equation for the covariances $\rho(x, x') = \langle\phi(x)\phi^*(x')\rangle$ because high-order correlations are not involved. Equations for these high-order correlations could also be obtained. However, this is not necessary if we wish to determine the averages of bilinear functionals such as

$$\mathcal{A} = \int A(x, x')\phi(x')\phi^*(x) dx dx'. \quad (21)$$

Its average is obtained from $\rho(x', x)$ by

$$\langle\mathcal{A}\rangle = \int A(x, x')\rho(x', x) dx dx'. \quad (22)$$

Equation (19) is the fundamental equation that we wished to derive. From this fundamental equation, we obtain the quantum Liouville equation and the Schrödinger equation by choosing a noise that changes the phase of $\phi(x)$ but not its absolute value. This is accomplished by choosing $G(x, x') = \gamma\delta(x - x')$. In this case, the terms of the Eq. (19) involving G vanish, and the equation is reduced to the equation

$$i\mu \frac{\partial}{\partial t} \rho(x, x') = \int [H(x, y)\rho(y, x') - \rho(x, y)H(y, x')] dy, \quad (23)$$

which is the quantum Liouville equation, if we replace μ by \hbar .

It is easily seen that the quantum Liouville Eq. (23) admits solutions of the type

$$\rho(x, x') = \psi(x)\psi^*(x'). \quad (24)$$

called pure states. If we replace this expression in (23), we found that this form is indeed a solution as long as $\psi(x)$ obeys the equation

$$i\mu \frac{\partial}{\partial t} \psi(x) = \int H(x, x')\psi(x') dx', \quad (25)$$

which is identified as the Schrödinger equation, if replace μ by \hbar . In other words, the Schrödinger equation is a particular case of the quantum Liouville Eq. (23) which is obtained when the initial condition is of the pure state type $\rho_0(x, x') = \psi_0(x)\psi_0^*(x')$, if this is allowed by the physical conditions. To avoid confusion with the wave function $\phi(x)$, which is a stochastic variable, we call $\psi(x)$ the Schrödinger wave function.

It is worthwhile writing down the equation that gives the time evolution of the average $\sigma(x) = \langle\phi(x)\rangle$ of the wave function $\phi(x)$. It is obtained by taking the average of (10), and the result is

$$\frac{d\sigma(x)}{dt} = \frac{1}{i\mu} \int H(x, y)\sigma(y) dy - \frac{1}{2} \int K(x, y)\sigma(y) dy \quad (26)$$

If the noise changes only the phase of $\phi(x)$, then we have $K(x, x') = \gamma^2\delta(x - x')$ and

$$\frac{d\sigma(x)}{dt} = \frac{1}{i\mu} \int H(x, y)\sigma(y) dy - \frac{1}{2}\gamma^2\sigma(x). \quad (27)$$

We remark that in the long run, σ vanishes and cannot be identified with the Schrödinger wave function ψ , which obeys the Schrödinger Eq. (25).

We point out that in accordance with the present approach the Eq. (19) as well as the quantum Liouville Eq. (23) and the Schrödinger Eq. (25) that follows from (19) are equations for the covariances $\rho(x, x') = \langle\phi(x)\phi^*(x')\rangle$ of the stochastic wave equation $\phi(x)$. In particular,

$\rho(x, x) = \langle |\phi(x)|^2 \rangle$ is the variance of the stochastic variable $\phi(x)$ which in the case of pure states is

$$|\psi(x)|^2 = \langle |\phi(x)|^2 \rangle \quad (28)$$

and, in view of the normalization (20), obeys the normalization

$$\int |\psi(x)|^2 dx = 1. \quad (29)$$

In accordance with the present approach, the variable x is a continuous parameter of the wave function, and $|\psi(x)|^2$ is the covariance of the wave function. The variable x is not properly a random variable. However, in view of the normalization (29), $|\psi(x)|^2$ is understood in the usual interpretation of quantum mechanics as the probability density distribution of x .

The equations that we have derived can be written in a more compact and familiar form by defining the operators associated with a bilinear function such as that given by (21). We define the operator \hat{A} acting on the vector space by

$$\hat{A}\phi(x) = \int A(x, x')\phi(x')dx'. \quad (30)$$

so that the bilinear functional \mathcal{A} is

$$\mathcal{A} = \int \phi^*(x)\hat{A}\phi(x)dx \quad (31)$$

In terms of the operators \hat{H} , $\hat{\rho}$ and \hat{G} associated with $H(x, x')$, $\rho(x, x')$, and $G(x, x')$, the Eq. (19) acquires the form

$$\frac{\partial \hat{\rho}}{\partial t} = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}] + \hat{G}\hat{\rho}\hat{G}^\dagger - \frac{1}{2}\hat{G}^\dagger\hat{G}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{G}^\dagger\hat{G}, \quad (32)$$

which has the form of the Lindblad equation for open quantum systems [20, 21]. We point out that $\text{Tr}\hat{\rho} = 1$, which follows from (20), and that $\langle \mathcal{A} \rangle = \text{Tr}\hat{A}\hat{\rho}$, which follows from (22). The quantum Liouville Eq. (23) and the Schrödinger Eq. (25) acquire the familiar forms

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}] \quad (33)$$

and

$$i\hbar \frac{\partial \psi(x)}{\partial t} = \hat{H}\psi(x), \quad (34)$$

In the case of pure states, that are solutions of the Schrödinger equation, the average $\langle \mathcal{A} \rangle$ is reduced to

$$\langle \mathcal{A} \rangle = \int \psi^*(x)\hat{A}\psi(x)dx \quad (35)$$

which is the familiar form for the quantum average of an observable.

The Schrödinger Eq. (25) is formally identical to the Eq. (8), and thus, the Schrödinger wave function $\psi(x)$ can be understood as related to the coordinate and momentum of the underlying classical system described by the classical Hamiltonian (5) which is now written in terms of ψ as

$$\mathcal{H} = \int \psi^*(x)H(x, x')\psi(x')dx dx'. \quad (36)$$

The question that now arises is how to describe the position and momentum of the quantum particle in terms of the coordinates and momenta of the underlying classical system, which are the real part and imaginary parts of ψ , respectively.

We start by assuming that the position \mathcal{X} of the quantum particles is given by

$$\mathcal{X} = \int \psi^*(x)x\psi(x)dx. \quad (37)$$

In accordance with (31), the corresponding operator \hat{x} is such that $\hat{x}\psi(x) = x\psi(x)$. Also, in accordance with (31), the momentum \mathcal{P} is of the form

$$\mathcal{P} = \int \psi^*(x)\hat{p}\psi(x)dx. \quad (38)$$

To determine the momentum \mathcal{P} , we regard it as the canonical conjugate to the position \mathcal{X} and should then be related by the Poisson commutation of the type $\{q, p\} = i\mu$, that is, $\{\mathcal{X}, \mathcal{P}\} = i\mu$. Replacing \mathcal{X} and \mathcal{P} given by (37) and (38) in the expression (3) for the Poisson brackets, we find

$$\{\mathcal{X}, \mathcal{P}\} = \int \psi^*(x)[\hat{x}, \hat{p}]\psi(x)dx. \quad (39)$$

Therefore, the following expression

$$\int (\psi^*(x)x\hat{p}\psi(x) - \psi^*(x)\hat{p}x\psi(x))dx = i\mu \quad (40)$$

should be fulfilled for an arbitrary function $\psi(x)$. This is accomplished if we choose \hat{p} to be the differential operator

$$\hat{p}\psi(x) = -i\mu \frac{\partial}{\partial x}\psi(x). \quad (41)$$

The Hamiltonian $\mathcal{H} = \mathcal{K} + \mathcal{V}$ is a sum of the kinetic energy \mathcal{K} plus the potential energy \mathcal{V} , which is expressed by

$$\mathcal{V} = \int \psi^*(x)V(x)\psi(x)dx. \quad (42)$$

To find the expression for the kinetic energy, we used the relation $\{\mathcal{X}, \mathcal{K}\} = \mathcal{P}/m$, where m is the mass of the quantum particle, from which follows that the respective operators are

related by $[\hat{x}, \hat{K}] = \hat{p}/m$. Therefore, we may conclude that $\hat{K} = \hat{p}^2/2m$ and that

$$\hat{H} = \frac{\hat{p}^2}{2m} + V. \quad (43)$$

Replacing this result in (34) and taking into account that \hat{p} is given by (41), we reach the equation

$$i\mu \frac{\partial \psi}{\partial t} = -\frac{\mu^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi, \quad (44)$$

which is the original equation introduced by Schrödinger.

In summary, we have derived the Schrödinger equation from the equations of motion of a classical underlying system with many degrees of freedom. The classical system is represented in a complex phase space whose components which are the dynamic variables are identified as the wave function $\phi(x)$. This complex phase space turns out to be a Hilbert space since the motion of the underlying classical system preserves the norm of $\phi(x)$. The probabilistic character of quantum mechanics is introduced by turning the wave function ϕ a stochastic variable, which is accomplished by adding a noise to the Hamilton equations, that preserves the the norm of $\phi(x)$.

From these assumptions, we derived a general equation for the covariances $\rho(x, x')$ of $\phi(x)$ that turns out to be of the Lindblad form. When the noise changes the phase of $\phi(x)$ but not its absolute value, this equation turns out to be the quantum Liouville equation for $\rho(x, x')$. A special type of solution of the quantum Liouville equation is of the type $\rho(x, x') = \psi(x')^* \phi(x)$. When this happens, $\psi(x)$ obeys an equation which turns out to be the Schrödinger equation.

The present approach to the Schrödinger equation does not reduce the science of quantum mechanics into the science of classical mechanics as the underlying classical system is not an observable. But the present approach allows for an interpretation of the wave function different from the standard interpretation [22–24]. Taking into account that the classical underlying system is a collection of interacting harmonic oscillator, the motion of the system can be understood as a wave motion, fitting the de Broglie ideas about quantum motion [25]. As the trajectory in the Hilbert space is stochastic, enabling several trajectories, it may also fit the consistent historical interpretation of quantum mechanics [6].

Declarations

Conflict of Interest The author declares no competing interests.

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