*ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА*
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# STOCHASTIC VARIATIONAL QUANTIZATION AND MAXIMUM ENTROPY PRINCIPLE

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In this paper, we discuss the stochastic variational method (SVM) to derive the action principle of Schrödinger equation. In this formalism, the wave function is introduced as one of convenient ways to express the action. This work is a reformulation of Nelson–Yasue's stochastic quantization scheme and its variational formulation by Yasue; it will furnish the possible way to deal with a more complicated system, such as quantum field theory, suggesting an origin of quantum mechanics.

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## 1. SINGLE PARTICLE MOTION

**1.1. Hydrodynamic Form of Action.** As is well-known, when we describe nonrelativistic motion of a particle under the influence of a potential $V$ in the form of variational principle, we take the coordinate vector $\mathbf{r}$ as its dynamical variable, and the variational principle is

$$\delta I_P \equiv \delta \int_{t_i}^{t_f} dt \ \left\{ \frac{m}{2} \left( \frac{d\mathbf{r}}{dt} \right)^2 - V(\mathbf{r}) \right\} = 0, \tag{1}$$

where $m$ is the mass, and the variation is taken with respect to an arbitrary variation of the trajectory, satisfying the boundary condition at $t_i$ and $t_f$. Of course, the Euler–Lagrange equation results in the equation of motion:

$$m \frac{d}{dt} \left( \frac{d\mathbf{r}}{dt} \right) = -\nabla V. \tag{2}$$

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The same problem can be also described in a different form. Let us now consider a set of infinite number of identical systems, each of them having different boundary (initial and final) conditions. These boundary conditions are given as in the form of initial and the final distribution of the particle positions. Then, to describe the dynamics of this ensemble (that is, the time evolution of the distribution of the flow of infinite particles), we can choose the density $\rho(\mathbf{r}, t)$ and the velocity field, $\mathbf{v}(\mathbf{r}, t)$ as dynamical variables. To write the equation of motion for this fluid in the form of variational principle, we can take the following action for $\rho(\mathbf{r}, t)$ and $\mathbf{v}(\mathbf{r}, t)$:

$$I_{\mathrm{CF}}[\rho, \mathbf{v}, \lambda] = \int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m\rho\mathbf{v}^2 - nV + \kappa\lambda(\mathbf{r}, t) \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\mathbf{v}) \right] \right\}, \tag{3}$$

where the last term in the integrand takes into account the dynamical constraint (continuity equation), $\partial\rho/\partial t + \nabla \cdot (\rho\mathbf{v}) = 0$, and $\lambda(\mathbf{r}, t)$ is an arbitrary adimensional field (Lagrangian multiplier). For convenience, the constant $\kappa$ with the dimension $[ET]$ is introduced to make $\lambda$ as adimensional. The variation of Eq. (3) should be taken with respect to $\rho, \mathbf{v}$, and $\lambda$.

The variation with respect to $\mathbf{v}$ gives the relation $m\mathbf{v} - \kappa\nabla\lambda = 0$, or

$$\mathbf{v} = \frac{\kappa}{m} \nabla\lambda, \tag{4}$$

that is, $\lambda$ is the velocity potential of the fluid. Note that $\mathbf{v}$ is necessarily irrotational (noninteracting dust).

Taking the variation with respect to $\rho$ and using the relation (4) to eliminate $\lambda$, then taking gradient of the resultant equation, we arrive at

$$\frac{\partial}{\partial t}\mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{m}\nabla V. \tag{5}$$

This is the Euler equation for the hypothetical "fluid", the ensemble of particles (dust). For a given initial condition, $\rho_0(\mathbf{r})$ and $\mathbf{v}_0(\mathbf{r})$, we can obtain the time evolution of the system by solving Eq. (5) together with the continuity equation. In particular, in this case, the left-hand side of the above equation is exactly the Lagrangian (total) derivative so that Eq. (5) reduced to Eq. (2).

**1.2. Action with Complex Amplitude.** The above variational action $I_{\mathrm{CF}}[\rho, \mathbf{v}, \lambda]$ for the flow of statistical ensemble of particles can be simplified by substituting Eq. (4) into the action as

$$I_{\mathrm{CF}}[\rho, \mathbf{v}, \lambda] \to I_{\mathrm{CF}}[\rho, \lambda] = \int dt \int d^3\mathbf{r}\, \rho \left\{ -\frac{\kappa^2}{2m}(\nabla\lambda)^2 - V - \kappa\dot{\lambda} \right\}. \tag{6}$$

Now, instead of the two scalar variables $(\rho, \lambda)$, let us introduce the complex amplitude,

$$\psi = \sqrt{\rho}\,\mathrm{e}^{i\lambda}, \quad \psi^* = \sqrt{\rho}\,\mathrm{e}^{-i\lambda}. \tag{7}$$

This is simply a different mathematical representation of the same degrees of freedom (see the later discussion). Therefore, we can re-express the action in terms of $\psi$ instead of $\rho$ and $\lambda$ as

$$I_{\mathrm{CF}}(\rho, \lambda) = \int dt \int d^3\mathbf{r}\ \psi^* \left\{ i\kappa \frac{\partial}{\partial t} - \bar{H} \right\} \psi, \tag{8}$$

where

$$\bar{H} = -\frac{\kappa^2}{2m}\nabla^2 + V - \frac{\kappa^2}{2m}(\ln\sqrt{\rho})^2. \tag{9}$$

Note that, from Eq. (6) to Eq. (8), partial integrations were introduced and the boundary condition has been used to eliminate surface terms.

## 2. INTRODUCTION OF NOISES

If we set $\kappa = \hbar$, the action given by Eq. (8) resembles that of the well-known Schrödinger equation, except for the additional term $\Delta U \equiv -\kappa^2(\nabla \ln\sqrt{\rho})^2/2m$. Of course, we will not arrive at quantum mechanics for free by a simple change of variables from the classical mechanics. The presence of the last term in the potential is fundamental since there should be an extra force which depends on the state of the ensemble ($\rho$ dependence).

Inversely, if we encountered some reasonable physical process which generates, for example, an additional internal energy part to increase the amount $-\Delta U$ which would cancel out the last term in Eq. (9), we would expect to have the same effect as quantum mechanics.

There are several real physical processes which increase the kinetic energy of a particle, such as thermal environment. In this section, we will try to incorporate the stochastic process into the variational formulation described above. The probabilistic form is particularly appropriate if the environment is really like thermal bath. There, the trajectory of a particle is constantly disturbed by the noise in the microscopic level. In a certain coarse-grained time scale, the trajectory appears completely zigzag Brownian motion, and each single event is never reproducible even if the initial condition is equally specified.

**2.1. Forward Stochastic Motion.** In the Brownian motion, let $\mathbf{u}_F$ define as the mean velocity of particles found at $\mathbf{r}$ at the time $t$. Then the position after an infinitesimal (but finite) time interval $dt$ is determined by the forward stochastic differential equation (FSDE):

$$d\mathbf{r} = \mathbf{u}_F(\mathbf{r}, t)dt + \boldsymbol{\xi}_F, \quad dt > 0, \tag{10}$$

where $\boldsymbol{\xi}_F$ is the Gaussian white noise with the width $\sigma^2 = \nu|dt|$, where $\nu$ is a constant having the dimension of $L^2/T$.

The probability density $\rho$ of finding a particle at the position $\mathbf{r}$ at time $t$ is defined as

$$\rho_F(\mathbf{r}, t) = \langle \delta(\mathbf{r} - \mathbf{r}(t)) \rangle_F, \tag{11}$$

where $\langle O(t) \rangle_F$ represents the average of $O$ at the instant $t$ over the whole events of the ensemble obeying the FSDE (10). The Fokker–Planck equation, corresponding to the stochastic differential Eq. (10), is

$$\frac{\partial \rho_F}{\partial t} + \nabla \cdot \mathbf{j}_F = 0, \tag{12}$$

where $\mathbf{j}_F = \rho_F(\mathbf{u}_F - \nu \nabla \ln \rho_F)$. Equation (12) is nothing but the continuity equation with the current containing the diffusion term due to the stochastic motion. This equation could be solved forward in time as the initial value problem if we knew $\mathbf{u}_F$. However, different from the case without stochastic disturbance, the solution obtained in this way does not fit the variational scheme, since the final state cannot be controlled in FSDE.

**2.2. Backward Stochastic Motion.** One possible way to control the final state, we think of stochastic process backward in time. That is, instead of the forward SDE (10), we introduce the time reversed SDE (BSDE):

$$d\mathbf{r} = \mathbf{u}_B(\mathbf{r}, t)dt + \boldsymbol{\xi}_B, \quad dt < 0, \tag{13}$$

where $\boldsymbol{\xi}_B$ is again the Gaussian noise. We further assume that there is no correlation between $\boldsymbol{\xi}_F(t)$ and $\boldsymbol{\xi}_B(t)$.

The probability density corresponding to BSDE $\rho_B\,(\mathbf{r}, t)$ can also be defined in an analogous form of Eq. (11), replacing the expectation value over the forward stochastic events by that of the backward ones. The Fokker–Planck equation for the time variation for the probability density equation, corresponding to the stochastic differential Eq. (13), is

$$\frac{\partial \rho_B}{\partial t} + \nabla \cdot \mathbf{j}_B = 0, \tag{14}$$

where $\mathbf{j}_B = \rho_B(\mathbf{u}_B + \nu \nabla \ln \rho_B)$. This equation can be solved from a given final condition in the backward direction in time $t$ for a given velocity field $\mathbf{u}_B = \mathbf{u}_B(\mathbf{r}, t)$. However, again, due to the presence of diffusion term in Eq. (14), this equation alone does not fit the variational scheme, since now the initial state cannot be controlled.

**2.3. Maximum Entropy Principle.** In 1966, Nelson [1] introduced the concept of the backward stochastic process to derive the Schrödinger equation. This approach is known as Nelson's stochastic quantization method. Later, Yasue [2] reformulated this idea in the form of optimization for the stochastic variables, known as stochastic variational method (SVM). Several applications of Yasue's SVM have been found in [3]. In this work, keeping the basic idea of deriving the quantum dynamics as a consequence of the two stochastic processes, we present an alternative representation of the quantization in the framework of variational method.

As pointed out, in order to formulate the variational approach, we have to consider both of the stochastic processes at the same time. For this, first, let us consider the number of trajectories obeying FSDE in a small space-time domain at $(\mathbf{r}, t)$. This naturally should be proportional to $\rho_F(\mathbf{r}, t)$ by definition. On the other hand, the number of trajectories in this domain which are obeying BSDE is proportional to $\rho_B(\mathbf{r}, t)$. Therefore, the number of possible combinations of trajectories which satisfy the both boundary conditions should be proportional to the product, $N(\mathbf{r}, t) \propto \rho_F(\mathbf{r}, t)\rho_B(\mathbf{r}, t)$. Now we require that the quantum mechanical law emerges when this combined number is maximum. In other words, the nature we observe is in a kind of statistical equilibrium, where the entropy $S = \int d^3\mathbf{r}\, N \ln N$ associated to connect the two trajectories is maximum. Since $\rho_F$ and $\rho_B$ are normalized, one can easily show that $\delta S = 0$ leads to

$$\rho_F(\mathbf{r}, t) = \rho_B(\mathbf{r}, t) \equiv \rho(\mathbf{r}, t). \tag{15}$$

The above requirement does not yet determine the dynamics of $\rho(\mathbf{r}, t)$. As we mentioned, $\rho(\mathbf{r}, t)$ satisfies the Fokker–Planck equations (12), (14), which still contain unknown velocity fields, $\mathbf{u}_F$ and $\mathbf{u}_B$. To obtain equations for these fields, we introduce the action principle. For combined fluids, it is reasonable to take the translational velocity as the average of these two velocities. Another linearly independent component, the relative velocity, would contribute to the internal energy of a fluid element. Thus, we take the action as simply the fluid action of the two velocities, one contributing to the translational kinetic energy, another to the internal energy as

$$I[\rho, \mathbf{u}_F, \mathbf{u}_B] \rightarrow \int dt \int d^3\mathbf{r}\rho \left[\frac{1}{2}m\left(\frac{\mathbf{u}_F + \mathbf{u}_B}{2}\right)^2 - V - \frac{1}{2}m\left(\frac{\mathbf{u}_F - \mathbf{u}_B}{2}\right)^2\right]. \tag{16}$$

As in the case of classical fluid, in addition to Eq. (16), the Fokker–Planck equations (12), (14) should be incorporated as constraints. To do so, using Eq. (15) and by adding the two Fokker–Planck equations (12) and (14), we obtain first the continuity equation $\partial_t \rho + \nabla \cdot (\rho \mathbf{u}_M) = 0$, where $\mathbf{u}_M = (\mathbf{u}_F + \mathbf{u}_B)/2$. On the other hand, the subtraction of the two equations leads to

$$\nabla \cdot (\mathbf{u}_F - \mathbf{u}_B - 2\nu \nabla \ln \rho) = 0. \tag{17}$$

The general solution of the above equation is $\mathbf{u}_Q = 2\nu\nabla \ln \rho + \nabla \times \mathbf{A}$, where $\mathbf{A}$ is an arbitrary time-dependent vector field [3]. In the presence of $\mathbf{A}$, the velocity field should contain a vortex which leads to a singularity in space. Here, for simplicity, we assume $\mathbf{A} \equiv 0$.

$$\mathbf{u}_F - \mathbf{u}_B = 2\nu \nabla \ln \rho, \tag{18}$$

which is called the consistency condition [2, 3].

As was done before, we can use Eq. (18) as constraint to reduce the variables in the action. Then we obtain

$$I[\rho, \mathbf{u}_M, \lambda] = \int dt \int d^3\mathbf{r}\, \rho \left[ \left\{ \frac{1}{2} m \left( \mathbf{u}_M^2 - \nu^2 \left( \nabla \ln \sqrt{\rho} \right)^2 \right) - V \right\} - \right. \\ \left. - \kappa \{ \dot{\lambda} + \nabla \lambda \cdot \mathbf{u}_M \} \right].$$

By requiring $\kappa = m\nu = \hbar$, the internal energy exactly cancels out the extra term in Eq. (9). Now, following the same procedure as in Sec. 1, we obtain

$$I[\rho, \mathbf{u}_M, \lambda] \to I[\rho, \lambda] = \int dt \int d^3\mathbf{r}\, \psi^*(\mathbf{r}, t) [i\hbar \partial_t - \hat{H}] \psi(\mathbf{r}, t), \tag{19}$$

where, as before, $\psi(\mathbf{r}, t) \equiv \sqrt{\rho}\, e^{i\lambda}$. The operator,

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}), \tag{20}$$

is exactly the usual form of Hamiltonian operator for a particle of mass $m$ in a potential $V(\mathbf{r})$. Naturally, the variation of the action Eq. (19) leads to the Schrödinger equation:

$$(i\hbar \partial_t - \hat{H})\, \psi(\mathbf{r}, t) = 0. \tag{21}$$

## 3. CONCLUDING REMARKS

The stochastic variational method introduced by Yasue [2] is formulated in "Lagrange picture" of fluid dynamics, that is, we consider the variation directly for the stochastic trajectory of quantum particles. In this work, we reformulate the same approach in a kind of "Euler picture" where the probability density $\rho$ is given by the maximum entropy state to make combinations of FSDE and BSDE. We show that the usual quantum mechanical action can be derived from the action corresponding to such a fluid which is composed of two velocity fields. In other words, our formulation indicates that quantum mechanic laws appear only when the entropy (number of combinatorial processes) associated with the above combination of FSDE and BSDE becomes maximum.

Application of the present formulation for the quantization of scalar field is rather straightforward [4]. As pointed out, the velocity in the present formulation is irrotational if $\lambda$ is a regular function. As was pointed out by Takabayashi and Wallstrom, the usual hydrodynamic representation of the Schrödinger equation cannot treat the cases where the phase of wave functions becomes multivalued [5]. However, for the field quantization, the vorticity in question refers to with the flow in the functional space. For the case of scalar field, the flow in the functional space can be taken always irrotational as in the case of one-dimensional harmonic oscillator. If the present formulation is the correct path of quantization of fields, the origin of quantum fluctuation should be directly related to the property of space and time. In other words, the origin of quantum mechanics can be intrinsically related with the emergence of space-time itself and then we would need to reconsider the meaning of quantization of gravity.

Another aspect of our formulation is that the Brownian motion is essential in the derivation of quantum mechanics as stochastic processes. This suggests the existence of the central limit theorem behind some unknown noises which are not necessarily to be the Wiener process.

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