Notes on the nonlinear nonlocal "Schrödinger equation" [1]

Alex A. Samoletov*

Institute for Physics and Technology, Natl. Acad. Sci. Ukraine, 340114 Donetsk, Ukraine

Abstract

It is shown that the nonlinear nonlocal equation [1] recently numerically studied in the context of quantum mechanics by Filippov is in fact a modification of the quantum-mechanical variational principle. It is shown that the result of Letter [1] admits clear analytical reading.

*E-mail: samolet@host.dipt.donetsk.ua

0. In a recent Letter [1] Filippov has presented a numerical study of nonlinear nonlocal "Schrödinger equation" in the context of quantum mechanics. In the present letter I intend to point out first, that in fact this equation is the result of a modification (generalization) of the quantum-mechanical variational principle, and, second, that there is clear analytical reading of the results of Letter [1].

I wish to express gratitude to A.Filippov for the possibility to read the manuscript of the Letter [1] before a publication as well as for demonstration of the results of numerical simulations.

The present letter to be considered as a continuation of Letter [1].

1. To begin with, I wish to make some preliminary remarks about the known facts [2], which are needed to the following.

Let us consider the Fokker-Planck equation for a scalar field $\psi(x)$ (generally, x take on values in $\mathbf{R}^d$, but, for the sake of brevity, the one-dimensional notation is taken)

$$\frac{\partial}{\partial t}P[\psi] = \int dx \frac{\delta}{\delta\psi(x)}\left[\left(\frac{\delta F[\psi]}{\delta\psi(x)} + \frac{\delta}{\delta\psi(x)}\right)P[\psi]\right], \tag{1}$$

where $t \in [0, \infty)$ is a (fictial) time. This equation has equilibrium solution of the form

$$P_\infty \sim \exp(-F[\psi]). \tag{2}$$

The functional P_∞ reaches its maximum value at a set of function which is associated with minimum of the functional $F[\psi]$.

Stochastic equation, which is stochastically equivalent to the Eq.(1), has the form

$$\frac{\partial}{\partial t}\psi(x,t) = -\frac{\delta F[\psi]}{\delta\psi} + \xi(x,t), \tag{3}$$

where $\xi(x,t)$ is the standard δ-correlated Gaussian field with the following averages

$$< \xi(x,t) >= 0, \qquad < \xi(x,t)\xi(x',t') >= 2\delta(x-x')\delta(t-t').$$

Eq.(1) with equilibrium solution (2) to be obtained from stochastic Eq.(3) as a result of averaging over all realizations of the random field $\xi(x,t)$. If we have a unique realization of the field $\xi(x,t)$, *as this happens to be the case for any numerical simulation*, and under a restriction on the functional F, then the system to be relaxed to the set of function on which a local minimum of the functional F has been realized. And then a formation of the equilibrium solution P_∞ to be started as the result of averaging in time. Next, after a

sufficiently large time t and on account of unlimited variation of the random field $\xi(x,t)$, the field $\psi(x,t)$ and a value of the functional F to be hustled away the minimum of F. Next, once again, the system (field ψ) to be relaxed, and so on, and so forth. Solution P_∞ will be formed at $t \to \infty$.

Thus, it is clear what the qualitative behavior of Eq.(3) solution to be expected. And we are now in a position to state and to solve the basic problem of the letter: Construction of a functional F which is needed to solution of Schrödinger equation.

Further we will consider only those systems whose evolution is given by the stochastic equation of the form (3).

2.Let H be a selfadjoint operator (Hamiltonian) and H is defined in Hilbert space $\mathcal{H}$, and let $\mathcal{H}$ is realized as $\mathcal{L}^2(\mathbf{R}^d)$; $\psi \in \mathcal{L}^2(\mathbf{R}^d)$. Let the quadratic form $(\psi, H\psi)$, where $(\cdot,\cdot)$ denote the scalar product in $\mathcal{H}$, be bounded below: $(\psi, H\psi) \geq \gamma(\psi,\psi)$. Then [3] the numerical range $\Theta(H)$ of H, otherwise speaking, a range of real numbers $(\psi, H\psi)/(\psi,\psi)$, be also bounded below. Closure of $\Theta(H)$ is the same as the convex hull of operator H spectrum $\Lambda(H)$ [3] and the greatest lower bound of $\Theta(H)$ coinsides with the greatest lower bound of $\Lambda(H)$ which is a ground state energy.

Consider now the eigenvalue problem: $H\psi = E\psi$, $(\psi,\psi) = ||\psi||^2 = 1$. As is well known, this problem is the same as the variational principle for functional

$$J[\psi] = (\psi, H\psi) + E||\psi||^2.$$

Thus, if we choose functional $F[\psi]$ of Eqs.(1)-(3) in the form $J[\psi]$, then the functional $P_\infty[\psi]$ has a minimum at the ground state and Eq.(3) has a unique attractor solution in case where H has a nondegenerate ground state.

In order that all eigenstates of H be search out, it is necessary to shift energy (numerical range of H) in positive direction of real axis. It is clear that this shift must be dependent on "time" t and functionally on ψ. Then, for each of $\psi(t)$ we shall have as a local attractive solution of Eq.(3) a lowest eigenstate depending on the value $||\psi||^2$ at the "time" t.

In a set of admissible shifts of the form $H \to H + S[\psi]\cdot I$, where $S[\psi] > 0$ for all nonzero $\psi \in \mathcal{H}$, it is necessary to select a subset such that the functional $S[\psi]$ has unique global minimum. It is obvious that simplest form of $S[\psi]$ is the following

$$S[\psi] = \alpha||\psi||^2, \qquad \alpha > 0.$$

In the case when $S[\psi]$ has more than one local minimum the evolution of $\psi(t)$ to be assumed an additional structure: a competition between the attracting character of local

minima of the functional $||\psi||^2 S[\psi]$ must be arisen (see Refs. in [1]). Discussion of these interesting cases must be down separately.

Thus, if our purpose is to search out all eigenstates of H as local attractors for Eq.(3) then it is reasonable to take functional $F[\psi]$ in its simplest form

$$F[\psi] = (\psi, H\psi) + \lambda||\psi||^2 + \alpha||\psi||^4. \tag{4}$$

Since the field $\xi(x,t)$ has unlimited variation (in any sense) it follows that $||\psi||^2$ can takes on arbitrary values in positive semiaxis. Hence, all eigenstates of H are attainable as local attractors.

It remains only to verify that $F[\psi]$ Eq.(4) is the functional which is used in Letter [1]. In fact, it is easily verified directly, when H is the Schrödinger operator: $H = -\frac{1}{2}\Delta + V(x)$. Further discussion and simulation of solutions of Eq.(3) given in Letter [1] remain true.

3. As a result we have

1. Method for a solution of eigenstate problems for Schrödinger operators of of [1] is the generalization (modification) of the quantum-mechanical variational principle.

2. A fictitious time is used in this generalization, so there is no reason for corresponding equation to be referred to as the Schrödinger equation with the real time.

3. In applications the method of [1] can be of the same importance as the variational principle.

4. The time-dependent Ginzburg-Landau equation of a particular form (with a complicated $S[\psi]$ is the case of the particular importance.

References

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[3] P.R. Halmos, A Hilbert space problem book (Van Nostrand, Princeton, 1976).