A Quasi-Newtonian Approach to Bohmian Mechanics I: Quantum Potential

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RÉSUMÉ. Dans cet article, nous faisons des investigations sur des points de vue Bohmian de la théorie de quantum, spécialement sur les potentiels Bohme de quantum. Nous développons une image quasi-Newtonienne des mecaniques de Bohme. Nous montrons que pour arriver á la formulation de la mécanique de quantum, il n'est pas nécessaire de commencer par l'équation de Schrödinger. Nous obtenons aussi des formes fonctionnelles de quantum, sans recourir aux ondes fonctionnelles et á l'équation de Schrödinger. Finalement, nous discutons á propos de la structure conceptuelle de la théorie de quantum.

ABSTRACT. In this article, we investigate Bohm's view of quantum theory, especially Bohm's quantum potential, from a new perspective. We develop a quasi-Newtonian approach to Bohmian mechanics. We show that to arrive at Bohmian formulation of quantum mechanics, there is no necessity to start from the Schrödinger equation. We also obtain an equation that restricts the possible forms of quantum potential and determines the functional form of it without appealing to the wave function and the Schrödinger equation. Finally, we discuss about the significance of quantum potential in the conceptual structure of quantum theory.

1 Introduction

Quantum theory was developed in 1920's and it explained a multitude of phenomena, including the atomic spectra. It introduced concepts like

wave function, *operators*, and *eigenvalues*, but at the same time it under-
mined some of the well-cherished philosophical principles like *causality*.
In his 1952 papers [1], David Bohm introduced a formulation of quantum
theory that kept many concepts of the standard quantum mechanics and
yielded the same empirical results, but was *causal*. In particular, Bohm
introduced the concept of *quantum potential*, which could be taken as
the source of quantum novelties.

In this article we deal with the meaning and role of quantum poten-
tial in the quantum theory. We start from a quasi-Newtonian approach
and then we show that by introducing the 'quantum potential' concept
into the mechanics of particles, one can get the mathematical form of
quantum potential by imposing the requirement that the total energy
of ensemble be minimized. Also we show that one can get Bohm's ba-
sic equations without appealing to the *Schrödinger equation* and *wave
function*.

2   Bohmian interpretation of quantum mechanics

According to quantum mechanics, the time development of the wave
function of a one-particle system is described by the time-dependent
Schrödinger equation:

$$ i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi. \tag{1} $$

Using Bohm's suggestion [1], we write the complex wave function ψ in
the polar form:

$$ \psi(x,t) = R(x,t)\exp(iS(x,t)/\hbar) \tag{2} $$

in which $R \geq 0$. Replacing equation (2) into (1), the complex equation
(1) reduces to the following real equations:

$$ \frac{(\nabla S)^2}{2m} + V(x) - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} + \frac{\partial S}{\partial t} = 0 \tag{3} $$

$$ \frac{\partial R^2}{\partial t} + \nabla.(R^2\frac{\nabla S}{m}) = 0. \tag{4} $$

The equation (4) is the so-called continuity equation, which is written
in terms of R and S. The equation (3) is very similar to the Hamilton-
Jacobi equation of classical mechanics. Therefore, Bohm [1] suggested

that we take S as Hamilton's principal function and take the momentum and energy of the particle to be

$$p = \nabla S, \quad E = -\frac{\partial S}{\partial t}. \tag{5}$$

In this view, we can discuss about the path of the particle, like in classical mechanics, something not permissible in the Copenhagen interpretation of quantum mechanics. Since S describes the phase of the wave function, and in quantum mechanics the wave function is taken to be single-valued, thus S has to be single-valued, apart from an additive constant such as $2\pi n\hbar$ (n is integer). R is also taken to be single-valued. While S in the classical mechanics is a multi-valued auxiliary function [2, Sec. 2.2.2], [3, Chap. 10], in the *ordinary* Bohmian interpretation, it seems that, it has more share of physical reality, relative to the classical case. In other words, in quantum mechanics, apparently, S has a role in the dynamics of the particle [2, Chap. 3]. The expression

$$Q(x) = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} \tag{6}$$

in equation (3) is called quantum potential, and in the Bohmian interpretation it can explain the non-classical behaviors of particles, such as interference, barrier penetration, etc. In short, we can say that in the usual Bohmian interpretation, the particle is under the influence of R and S, in addition to the external potential $V(x)$. In this interpretation, one assumes the fundamental Schrödinger equation, but tries to extract another meaning from the wave function. The Bohmian mechanics, as we know it, is not usually taken to be a theory independent from the standard quantum theory. But it attempts to dispense with some of the interpretational aspects of quantum theory, such as indeterminism and the lack of particle trajectory. Like ordinary quantum mechanics, the fundamental element of the ordinary Bohmian mechanics is the wave function which develops according to the Schrödinger equation. But the phase and the amplitude of the wave function are interpreted in such a way that the concept of particle and its path remain intact. Even, if one finds cases which the predictions of the Bohmian mechanics and the ordinary quantum mechanics are different, this does not mean that we are dealing with two basically different theories. Because, when we interpret the elements of a theory (e.x. position and momentum) in a special manner and give special meaning to those elements, the method

of problem solving, and consequently, the predictions, could be affected. Therefore, that interpretation will be adopted which fits the empirical results better.

3   Quasi-Newtonian approach

If we look at the ideas of David Bohm [1], [4] we find that, his main purpose to develop the so-called Bohmian interpretation was to prove that the von Newmann's argument about the impossibility of describing the current quantum mechanics on the basis of 'Hidden variables' is wrong. He realized that by supposing a strictly well-defined localized particle with a well-defined trajectory that coexists with the wave and interpreting ∇S and $-\partial S/\partial t$ as momentum and energy of the particle that the Schrödinger wave function describes, we can consistently describe all known quantum phenomena. But, what he found was very powerful, specially in solving the measurement problem in the quantum mechanics [1], [2, chap. 8]. In the Bohmian interpretation it is very simple to show how the measurement process terminates with one of the eigenvalues of relevant quantum mechanical operator [2, chap. 8], without needing the collapse of the wave function. Therefore, one of the merits of including a localized particle with well-defined trajectory to the quantum theory is to reducing the number of postulates we need to describe quantum phenomena. This fact by itself is sufficient to show that the Bohm's trajectories are not some artificial curves added to a pre-existing quantum theory. In a subsequent paper we show that, even there is no need for postulating the 'eigenvalue postulate'. It is a natural consequence of Bohmian approach to *prove* that even prior to any measurement the energy and angular momentum of electron in the atom in stationary states are eigenvalues of relevant operators.

What is revolutionary, in the Bohm interpretation, in contrast to the Copenhagen interpretation of quantum mechanics? The answer absolutely is, 'causality' and 'trajectories'. In the Copenhagen interpretation, the only causal element is the evolution of wave function with time. There is no other causal element in that interpretation. Because of the lack of causality, the particles do not have any well-defined trajectories in space and time. In this respect, the Bohm's idea is revolutionary. In other words, in comparison with formulation of orthodox quantum mechanics, the Bohm's idea is revolutionary. In this viewpoint, the main part of Bohmian formulation of quantum mechanics is the equation $p = \nabla S$, by which we can *define* or *obtain* the particle's

trajectory. According to some authors, for interpreting ∇S as particle momentum, appealing to the modified Hamilton-Jacobi equation (3) is not a necessity. One can arrive at

$$\dot{x} = \frac{\hbar}{m} Im \frac{\nabla \psi}{\psi} = \frac{\nabla S}{m} \tag{7}$$

only by appealing to some symmetry arguments about the wave function itself [5],[6]. In this view, the only property of Bohm's particle is its position. This position evolves with time, according to (7). The wave function is responsible for the evolution of particle's position with time. It seems that, according to this viewpoint, there is no need for the Newtonian concepts such as energy, momentum, angular momentum, $\cdots$, for the particle. The particle has only a position that the evolution of which is determines strictly by the wave function.

As we mentioned, if we compare the Bohmian mechanics with the Copenhagen interpretation, the new revolutionary elements are the 'causality' and 'trajectories'. But, just these two elements are 'trivial' and 'no revolutionary', if we compare the Bohmian mechanics with classical (Newtonian or Einsteinian) mechanics. We should not forget that the classical mechanics is successful theory of the world around us. The presence of 'quantum phenomena' must not be the cause of disregarding the 'classical phenomena', such as the freedom of throwing a thing with arbitrary initial momentum, and the absence of interference phenomenon for particles.

Therefore, in comparison with classical mechanics, the main element of Bohmian mechanics is not the equation $p = \nabla S$. Indeed, whenever we have a Newtonian force equation like $dp/dt = -\nabla V$ or $dp/dt = -\nabla(V + Q)$(as we have from Bohm's formulation), we can find a S function such that we have $p = \nabla S$. This equation is a mathematical definition. Indeed, arriving at this relation by starting from a Newtonian force law is much simpler that arriving at it through symmetry considerations about the wave function. In this regard, the revolutionary parts of Bohmian mechanics are the presence of a highly non-classical potential, named quantum potential, and the Born rule -issues that are not independent, because both depend on function R. In the classical mechanics, there is neither quantum potential, nor the Born rule.

In this paper and subsequent papers, we try to develop a quasi-Newtonian approach to Bohmian mechanics.

3.1   Illustrating the quasi-Newtonian approach

In the quasi-Newtonian approach, we try to describe quantum phenomena in a manner nearest to the classical mechanics. Although the quantum phenomena are non-classical, we encounter them as some new regularities which had been hidden. They are rules of nature which do not make manifest themselves in the daily experiences.

One of the most important quantum phenomena is two slit interference. When a flux of identical particles passes from two slits and reaches a screen, it shows a wave like dark-bright fringes, in the sense that the number density of particles on the screen differs from bright regions to dark regions. If we emit the particles one by one on the slits, after a long time the dark-bright pattern appear. This fact shows that the whole pattern is the result of the behavior of individual particles. If we believe that the behavior of individual particles in this experiments is essentially deterministic, we expect, in a quasi-Newtonian picture, that an extra potential must be responsible for this novel behaviors. The effect of this extra potential is such that prevents the particles to fall in dark regions and forces them to fall almost in the central regions of bright fringes.

If we denote the number density of the particles by ρ, and the apparent extra potential that acts on the individual particles by Q, and try to denote the mathematically unknown fundamental agent of these novel behaviors by χ we must have

$$\rho = f(\chi) \tag{8}$$

$$Q = Q(\chi). \tag{9}$$

But the Eq. (8) can not specifies ρ uniquely, because we can emit a flux with arbitrary intensity. Therefore, the total number of particles in the flux is arbitrary. Indeed, this equation must specifies the form of distribution of ρ in the space and on the screen. We can fix the exact values of ρ by specifying the value of ρ at a given point x_0 as ρ_0. Inserting this condition into (8), it must specify ρ uniquely. Another way for specifying ρ uniquely, is to specify the total number N of particles in the flux. This is accomplished by the relation

$$\int \rho \, d^3 x = N. \tag{10}$$

Dividing both sides of this relation by N, we can always obtain a normalized ρ such that

$$\int \rho \, d^3x = 1. \tag{11}$$

Suppose that we can mathematically get the inverse of the Eq. (8) in the form:

$$\chi = f^{-1}(\rho). \tag{12}$$

By this relation we can eliminate the unknown agent χ from the problem. Inserting this equation into (9) we obtain

$$Q = Q(\rho). \tag{13}$$

Note that the dependence of Q on ρ is not basically direct and is only a technic for solving the problem, by eliminating the unknown factor χ.

Conforming to the usual Bohmian mechanics formulation, we introduce a function R such that we have

$$\rho = R^2. \tag{14}$$

According to the usual formulation of Bohmian mechanics, one may think of R as being the amplitude of a wave function. But, we don't have any emphasis on R as being the amplitude of a wave function, and we can even show that this is not a good interpretation, because it would be suitable to allow negative values for R.

Due to (14) we can rewrite Eq. (13) as

$$Q = Q(R). \tag{15}$$

This equation means that Q could be function of R and its partial derivatives.

Now, We consider the Hamiltonian of a single particle in three dimensions:

$$H(x, p, t) = \frac{p^2}{2m} + V(x) + Q(R(x, t)) \tag{16}$$

where the quantum potential Q is taken to be unknown function of R. For the moment, we assume that the function R does not depend on time and therefore the energy is conserved in the presence of quantum potential Q . Therefore, the energy of particle is taken to be

$$E = H(x, p) = \frac{p^2}{2m} + V(x) + Q(R(x)). \tag{17}$$

Without knowing the functional dependence of Q with respect to R we are not able to solve the problem of finding the path of the particle. We need extra assumptions about R and Q. We appeal to a simple (or the simplest) assumption: the total energy of the ensemble of particles must be minimized.

This means that we minimize the integration

$$\int \rho H d^3 x \tag{18}$$

while keeping the condition (11). According to variations calculus, we can write this requirements as

$$\delta \int \rho \{H - \lambda\} d^3 x = 0 \tag{19}$$

in which λ is Lagrange's undetermined multiplier.

This equation is not useful unless we could write Hamiltonian completely as a function of space coordinates only. This is feasible by using Hamilton-Jacobi's principal function S. According to the Hamilton-Jacobi theory, we can express the momentum of particle as

$$p = \nabla S \tag{20}$$

and for conserved systems we have

$$S(x, t) = W(x) - Et. \tag{21}$$

Therefore, using the Eq. (20), we can express the Hamiltonian as a function of space coordinates only and rewrite Eq. (19) as

$$\delta \int R^2 \left\{ \frac{(\nabla S)^2}{2m} + V + Q - \lambda \right\} d^3 x = 0. \tag{22}$$

This equation is an eigenvalue problem with λ as eigenvalue. Therefore we call λ the energy eigenvalue. It is simple to prove that whenever the quantum potential Q is in the Bohmian form (6), λ is identical to eigenvalue of the time-independent Schrödinger equation (Appendix). In other words, the Eq. (22) is an integral form of the energy eigenvalues differential equation.

For the reasons, which will be explained later, we assume Q to be a function of R and its first and second derivatives. Indeed, we show that the insufficiency of first order derivatives and the presence of second derivatives is a necessity for the existence of non-trivial quantum potential.

If we denote the integrand of (22) by g, using summation rule for indices i, j and abbreviation ∂_i for the partial derivative $\partial/\partial x_i$, and so on, we have from variational calculus

$$\frac{\partial g}{\partial R} - \partial_i\left(\frac{\partial g}{\partial(\partial_i R)}\right) + \partial_i\partial_j\left(\frac{\partial g}{\partial(\partial_i\partial_j R)}\right) = 0 \qquad (23)$$

$$\partial_i\left(\frac{\partial g}{\partial(\partial_i S)}\right) = 0. \qquad (24)$$

From the equation (23) it follows that:

$$\begin{aligned} & 2R\left\{\frac{(\nabla S)^2}{2m} + V + Q - \lambda\right\} + \\ & R^2\frac{\partial Q}{\partial R} - \partial_i\left(R^2\frac{\partial Q}{\partial(\partial_i R)}\right) + \partial_i\partial_j\left(R^2\frac{\partial Q}{\partial(\partial_i\partial_j R)}\right) = 0. \end{aligned} \qquad (25)$$

The expression between braces is $E - \lambda$. Therefore, this equation reduces to

$$R^2\frac{\partial Q}{\partial R} - \partial_i\left(R^2\frac{\partial Q}{\partial(\partial_i R)}\right) + \partial_i\partial_j\left(R^2\frac{\partial Q}{\partial(\partial_i\partial_j R)}\right) = 2R\{\lambda - E\}. \qquad (26)$$

The quantity E is the particle energy, i.e., is a constant related to the particle dynamics. On the other hand, the energy eigenvalue λ is a constant related to the particle dynamics. Thus, it is natural to take them to be identical. Indeed, we seek cases where the energy of the particle is equal to the energy eigenvalue. Theoretically, there is the

possibility for the particle energy to be different from energy eigenvalues. But, we take them identical here. Therefore, we have

$$\lambda = E = \frac{(\nabla S)^2}{2m} + V(x) + Q \qquad (27)$$

$$R^2 \frac{\partial Q}{\partial R} - \partial_i (R^2 \frac{\partial Q}{\partial(\partial_i R)}) + \partial_i \partial_j (R^2 \frac{\partial Q}{\partial(\partial_i \partial_j R)}) = 0. \qquad (28)$$

Consequently, the equation (28) is an important condition that quantum potential Q must fulfill. From the equation (24), one gets

$$\nabla.(R^2 \frac{\nabla S}{m}) = 0 \qquad (29)$$

which is the so-called continuity equation for stationary states.

3.2   The derivation of the quantum potential

We have to find a function $Q(R)$ which satisfies the equation (28). The form of Q with respect to R must be such that the Eq. (28) is satisfied for every arbitrary R. Indeed, we do not have inclination that the condition (28) restricts the acceptable forms of R. Our interest is to restrict the functional form of Q with respect to R, not the form of R with respect to x. The simplest solution is

$$Q \equiv const \qquad (30)$$

in which, Q appears as an additive constant in the energy equation. This is satisfied for arbitrary R. If we did not have the equation (29), we could obtain from equation (30) the whole of classical mechanics, apart from a constant value in the energy. The condition (29) imposes some restrictions on the particle motion (such as prevention of turning points in the particle orbits, as we shall see in a subsequent paper) - conditions which are not imposed in the classical mechanics. Therefore, if we restrict ourselves to stationary states we can not describe the whole classical dynamics. To describe the whole classical dynamics we should consider equation (30) for non-stationary states. If the constant Q is non-zero, we should not, however, confuse this constant with the origin of potential energy in classical mechanics, as we have not made any changes in the origin of potential. Thus, a constant Q would be a real

non-classical term. If it is non-zero and dependent on the particle, one may interpret it as the rest energy, but there is no way to prove this.

Now, we can expect that more complicated forms of Q would lead to non-classical results. We are looking for a non-trivial expression for Q. Consider that, Q is a function of R and its first and second derivatives. We shall see a little later that the first-order derivatives are not sufficient for getting a non-trivial quantum potential. The quantum potential Q is a scalar function and therefore must be rotational-invariant. Thus, we expect that the first and second derivatives of R appear in the form of $|\nabla R|$ and $\nabla^2 R$, respectively. Therefore, Q is constructed from the factors $f_1 = R^m$, $f_2 = |\nabla R|^n$ and $f_3 = (\nabla^2 R)^p$ for some unknown powers m, n and p. Among all the expressions that one can write by summation or multiplication of these factors the only expression that leads to a non-trivial form for quantum potential is $f_1 f_2 f_3$, i.e.

$$Q = A\, R^m \, |\nabla R|^n \, (\nabla^2 R)^p. \tag{31}$$

We emphasize that *only expressions in the form of* (31) *lead to a non-trivial solution for equation* (28). Inserting the equation (31) into (28), one can show, after some elementary (but, to some extent long) calculations, that only two sets of values for m , n and p can lead to a satisfactory solution for the equation (28):

$$m = 0, \quad n = 0, \quad p = 0$$
$$m = -1, \quad n = 0, \quad p = 1.$$

In the first case, we get trivial solution $Q(x) = A = const$, which we have already discussed. The second case leads to the result that we have in ordinary Bohmian mechanics. We observe that with $p = 0$, the equation (28) can be satisfied for no values other than zero for m and n. Remembering that no expressions other than (31) can lead to a non-trivial solution for Q, we observe that the presence of a non-trivial solution for Q requires $p \neq 0$, i.e., it shows the necessity of second-order derivatives.

Thus, the simplest non-trivial form of the quantum potential is in the form

$$Q(x) = A\frac{\nabla^2 R}{R}. \tag{32}$$

This means that we not only got the quantum Hamilton-Jacobi equation and the continuity equation, but we also justified the form of Q in terms of R. Thus, if we are to have a quantum potential, its simplest non-trivial form is the familiar one. We observe that the form of quantum potential (32) is a mathematical necessity for minimizing the total energy of the ensemble rather than being a consequence of the Schrödinger equation. This shows the power of quantum potential concept in the quantum theory.

The constant value of A and specifically its sign in the equation (32) are significant. Any departure from the value of A that we get from quantum mechanics leads to serious changes in the particle dynamics. But, here we don't have any independent way for getting its value. It seems that the simplest way for obtaining the constant A is by adapting the energy levels of Hydrogen atom in the theory with those obtained from Bohr's model. This is exactly what Schrödinger did in his original works for finding some constants [7, p. 8]. We expect that this method yields the value $-\hbar^2/2m$ for A, and therefore we take it simply to be $-\hbar^2/2m$.

Note that in this discussion we have not made any use of the concept of wave function. Here S is a mathematical function, the derivatives of which gives momentum and energy, and R is representative of a new physical entity which contributes to the dynamics of the particle through Q.

This can means that quantum potential is a more fundamental concept than wave function and Schrödinger equation.

If the state is not stationary, i.e., R depends on time and S is a general function of time and space, we can directly use

$$\delta \int R^2 \left\{ H(x, S(x,t), R(x,t)) + \frac{\partial S}{\partial t} \right\} d^4x = 0 \qquad (33)$$

and the relations (23), (24) and (32), to obtain the Hamilton-Jacobi and continuity equations (here the index i includes time as well):

$$\frac{(\nabla S)^2}{2m} + V(x) + Q + \frac{\partial S}{\partial t} = 0 \qquad (34)$$

$$\frac{\partial R^2}{\partial t} + \nabla.(R^2 \frac{\nabla S}{m}) = 0. \tag{35}$$

Needless to say that the Eq. (22) is in fact a special case of the equation (33). If R is not an explicit function of time, and S is written in the form of (21), the time integration in equation (33) reduces to a multiplying constant, and therefore the equation (33) leads to the earlier result, i.e., the equation (22) with $\lambda = E$.

4 Relation with the usual Bohmian mechanics

In the previous section, We obtained the Bohmian equations of quantum theory from simple considerations, without starting from Schrödinger equation. Mathematically, the set of Eqs. (34) and (35) along with the condition

$$\oint \nabla S.dx = nh \tag{36}$$

is equivalent to the Schrödinger equation for $\psi = Re^{iS/\hbar}$. The condition (36) means that the phase of wave function is unique and thus the wave function is single-valued. Without this condition one can not consider S as phase of a wave function. Establishing this condition is equivalent to appealing to the wave function, and denying it means denying wave function in the theory.

In our approach, there is no need and no reason for imposing the condition (36). This means that we do not appeal to the wave function. This is a major difference between quasi-Newtonian approach and usual Bohmian mechanics. Indeed, in the quasi-Newtonian approach S is the same as classical Hamilton-Jacobi principal function: there is no uniqueness condition (36) on S.

Another difference between quasi-Newtonian approach and usual Bohmian mechanics is connected with the denial of the condition (36). When we do not need to consider the S as phase of a wave function there is no need to consider R as amplitude of a wave function. Therefore, there is no need to consider R as a positive-definite function. We know from usual Bohmian mechanics and also from our approach that R appears in the forms of R^2 or $\nabla^2 R/R$, thus negative values for R is not a problem. In a subsequent paper on 'quantization', we shall show that the

imposition of the uniqueness condition on S and the positive-definiteness condition on R are not necessary for solving quantum problems.

5   Conclusion

As we observed in this paper, one can start from a quasi-Newtonian approach and get the mathematical form of quantum potential by minimizing the total energy of ensemble, without appealing to the Schrödinger equation and wave function. This approach yields that the non-trivial quantum potential necessarily is in the Bohmian form. After the derivation of the mathematical form of quantum potential, if we impose the extra uniqueness condition on S (which is not necessary in quasi-Newtonian approach), one can obtain the Schrödinger equation. This means that one can consider the Bohmian quantum potential as the basis of the Schrödinger equation rather than being a consequence of it. In this picture, the quantum potential is the fundamental concept of quantum theory, because it provides for the classical mechanics the possibility of existing non-classical effects.

A

It is simple to prove that the equation (22) with Bohmian quantum potential (6) is an integral form of the time-independent Schrödinger equation. For stationary states we have

$$\psi^\star \hat{H} \psi = R^2 \left\{ \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \right\}$$

Using the quantum potential $Q = AR^{-1}\nabla^2 R$ with $A = -\hbar^2/2m$, equation (22) becomes

$$\delta \int \left\{ R^2 H - \lambda R^2 \right\} d^3 x = \delta \int \psi^\star \left\{ \hat{H}\psi - \lambda\psi \right\} d^3 x = 0$$

Variation with respect to $\psi^\star$ yields

$$\hat{H}\psi = \lambda\psi$$

that is time-independent Schrödinger equation with eigenvalue λ.

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