Maupertuis-Hamilton least action principle in the space of variational parameters for Schrödinger dynamics; A dual time-dependent variational principle

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Abstract

Time-dependent variational principle (TDVP) provides powerful methods in solving the time-dependent Schrödinger equation. As such Kan developed a TDVP (Kan 1981 Phys. Rev. A 24, 2831) and found that there is no Legendre transformation in quantum variational principle, suggesting that there is no place for the Maupertuis reduced action to appear in quantum dynamics. This claim is puzzling for the study of quantum–classical correspondence, since the Maupertuis least action principle practically sets the very basic foundation of classical mechanics. Zambrini showed within the theory of stochastic calculus of variations that the Maupertuis least action principle can lead to the Nelson stochastic quantization theory (Zambrini 1984 J. Math. Phys. 25, 1314). We here revisit the basic aspect of TDVP and reveal the hidden roles of Maupertuis-Hamilton least action in the Schrödinger wavepacket dynamics. On this basis we propose a dual least (stationary) action principle, which is composed of two variational functionals; one responsible for ‘energy related dynamics’ and the other for ‘dynamics of wave-flow’. The former is mainly a manifestation of particle nature in wave-particle duality, while the latter represents that of matter wave. It is also shown that by representing the TDVP in terms of these inseparably linked variational functionals the problem of singularity, which is inherent to the standard TDVPs, is resolved. The structure and properties of this TDVP are also discussed.

1. Introduction

We revisit the quantum mechanical time-dependent variational principle (TDVP) from the view point of the classical least action principles of Maupertuis and Hamilton. Much is already known about the quantum–classical correspondence up to the sophisticated studies on semiclassical mechanics [1–6]. Well-known relationships of quantum theories to classical counterparts are, for instance, the Schrödinger equation to the Hamilton-Jacobi equation [7], the Heisenberg equation to the Hamilton canonical equations of motion (the commutator to the Poisson bracket) [8], Wigner phase-space theory [3, 9] to the classical Liouville equation, Feynman path integrals [10] to the Lagrangian dynamics through the stationary state approximation [1], Nelson’s stochastic quantization [11] to the Newtonian equation, and so on. It is astonishing for both quantum and classical mechanics to have such a variety of seemingly different yet essentially equivalent forms. However, to the best of our knowledge, relationship between quantum theory and the least action principle of Maupertuis has not been well studied for a long time after the birth of quantum theory. Only in 1984, Zambrini [12] showed that Maupertuis’ principle of least action in the stochastic calculus of variations leads both to the Nelson stochastic quantization equation [11] and the Newtonian equation in the two opposite extrema. (The basic theory of the stochastic calculus of variations had been developed by Yasue [13]. For very recent progress in stochastic variational principle, see [6, 14, 15].) Being beautiful, the Nelson stochastic quantization is not necessarily useful in applications to multi-dimensional systems.
By contrast, the TDVP gives far more practical methodologies. Indeed, there have been proposed various elaborated formalisms such as those of the so-called Dirac-Frenkel, MaLachlan [16], Kan [17], Kramer and Saraceno [18], and so on. Broeckhove, Lathouwers, Kesteloot and van Leuven [19] gave a unified account over these methods. These methods and the variants are widely used in many fields of physics and chemistry. (For more recent progress in other general theories of TDVP, we refer to [20–26].) Yet, it is known that the TDVP generally faces a divergence problem in handling nonlinear variational parameters, which arises from the inversion of possibly singular matrices.

An overwhelming advantage of TDVP is that it transforms the Schrödinger partial differential equation to a set of coupled ordinary differential equations over the space of variational parameters. In this context, Kan [17] determinedly states in his seminal paper that ‘any time-dependent description of quantum systems derived from the variational principle is equivalent to Hamilton’s description of a classical system’. On the other hand, Kan has explicitly shown that there does not exist Legendre transformation in his TDVP. Lack of the Legendre transformation suggests that there is no place for the Maupertuis reduced (or abbreviated) action [27, 28] to appear, and therefore the Maupertuis–Hamilton least action principle will not have direct significance in TDVP. It is not comfortable however to accept this assertion, since the least action principle of Maupertuis and Hamilton sets a theoretical foundation of classical mechanics. Or more objectively, it serves as an axiom for classical mechanics, from which the entire structure of classical formalisms is deduced [27, 28]. We therefore reexamine the hidden roles of the Maupertuis least action principle in TDVP for the Schrödinger dynamics. [We are aware of Schwinger’s lecture about quantum action principle [8], discussing the parallelism between the Heisenberg equation and Hamilton canonical equations of motion. But this is a different story. Also, Karamatskou and Kleinert [29] developed a theory in which a Schrödinger wavefunction is to be propagated as a free wave moving through a curved space. This is an analogy to the Maupertuis principle asserting that the movement of a classical particle in an external potential can be regarded as a free movement in a curved space with the relevant metric. Yet, this theory has no direct relevance to the present work either.]

In the present study on TDVP, we draw two main conclusions. (1) One can introduce the Maupertuis–Hamilton least action principle into the space of quantum variational parameters. This principle is composed of twin variational functionals, one responsible for ‘energy related dynamics’ and the other for ‘dynamics of wave-flow’. From the view point of the wave-particle duality, the former is mainly a manifestation of particle nature, while the latter reflects the nature of matter wave. We refer to this variational method as dual least action principle. (2) By representing the TDVP in terms of two inseparably coupled variational conditions as above, the problem of singularity that is inherent to the standard TDVPs is resolved. We also demonstrate other features of the present TDVP such as the necessity of classification of variational parameters.

The rest of this paper resumes with a very brief summary of the well studied part of TDVP in section 2. We propose in section 3 a dual least action principle. The properties of the proposed variational functionals such as quantum flux in the space of variational parameters are also presented. In section 4 we discuss mathematical conditions that automatically nullify the variational functional with respect to the dynamics of wave-flow. This paper concludes with some remarks in section 5.

2. Preliminary for time-dependent variational principles

This section is devoted to a brief review for some basic variational principles which are particularly relevant to the present work. This section therefore includes no new material, and may be skipped to the next section.

2.1. Brief reminder of the classical least action principle

We first recall classical variational principle very briefly. The Lagrangian $L(q, \dot{q}, t)$ is supposed to satisfy

$$\delta \int L(q, \dot{q}, t) dt = 0$$

under the double ended boundary condition

$$[q\delta q]_{\text{end}}^{\text{end}} = 0.$$  

The the Euler–Lagrange equation of motion then follows as

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0.$$  

Further, using the Legendre transformation, the momentum coordinate $p$ is introduced, and the Hamiltonian is defined as
$H = p\dot{q} - L,$ \hspace{1cm} (4)

where $\int p\dot{q} \, dt$ is referred to as the Maupertuis reduced (abbreviated) action [27]. Then another form of the least action principle follows as

$$\delta \int (p\dot{q} - H) \, dt = 0,$$ \hspace{1cm} (5)

and one obtains the standard classic canonical equations of motion (with mass $m = 1$ in the mass-weighted coordinates)

$$\frac{d}{dt} q = \frac{\partial H}{\partial p} \hspace{1cm} \text{and} \hspace{1cm} \frac{d}{dt} p = -\frac{\partial H}{\partial q},$$ \hspace{1cm} (6)

where $(q, p)$ is a canonical conjugate pair of independent dynamical variables. Knowing difference between the Maupertuis principle and Hamilton principle, we here refer to equation (5) simply as the Maupertuis-Hamilton principle to stress the presence of the Maupertuis reduced action. Among the most important consequences from them are energy conservation along $(q(t), p(t))$ and the relevant absolute invariances for a time-independent Hamiltonian [28]. Thus, the classical Lagrangian and Hamilton are mutually convertible through the Legendre transformation. It is therefore noteworthy that Kan emphasized that such a Legendre transformation does not exist in his quantum TDVP [17].

We recall that the role of the term $pq\dot{}$ in the classical variational principle equation (5) is not limited to the Legendre transformation alone; It is of course needed to ensure energy conservation for time-independent Hamiltonians and is also known to be subject to the Poincaré-Cartan integral invariance [28]. We see later the similar situation in the quantum parameter space.

### 2.2. Dirac-Frenkel and Kan variational principles

#### 2.2.1. Dirac-Frenkel

We start with the Schrödinger equation

$$\left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi(t) = 0$$ \hspace{1cm} (7)

and try to find the solutions within a class of trial functions that satisfy variational condition

$$\delta \left\{ \phi \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi \right\} = 0.$$ \hspace{1cm} (8)

In the studies on dynamics of molecules, for instance, the following Gaussian-type wavepackets are frequently used for trial functions, which contain three classes of parameters

$$\phi(q, t) = N(t) \sum_{j} \left( c^{(0)}_{j}(t) + c^{(1)}_{j}(t)(q - q_{0j}(t)) + c^{(2)}_{j}(t)(q - q_{0j}(t))^{2} + \cdots \right) \times \exp \left( \frac{i}{\hbar} P_{0j}(t)(q - q_{0j}(t)) \right) \times \exp \left( - \left( \alpha_{j}(t) + i\beta_{j}(t) \right)(q - q_{0j}(t))^{2} + \cdots \right)$$ \hspace{1cm} (9)

Here the linear parameters $\{c^{(0)}_{j}(t), c^{(1)}_{j}(t), c^{(2)}_{j}(t), \cdots \}$ are supposed to be complex values and are responsible for shape deformation of the packets. The set of nonlinear parameters $\{q_{0j}(t), P_{0j}(t)\}$ generally represent the external motion or transport of each packet, while $\{\alpha_{j}(t), \beta_{j}(t), \cdots \}$ are supposed to describe the spatial broadening and oscillatory feature of the wavefunction. Note that the variational parameters are included implicitly in the normalization constant $N(t)$.

When a trial function includes only linear parameters in such a way that

$$\phi = \sum_{j} C_{j}(t) \chi_{j},$$ \hspace{1cm} (10)

where $\chi_{j}$s are generally complex-valued basis functions, equation (8) simply gives

$$i\hbar \frac{\partial}{\partial t} C_{j} = \sum_{k} \langle \chi_{k} | \hat{H} | \chi_{j} \rangle C_{j}.$$ \hspace{1cm} (11)

Thus it is readily confirmed that the linear variational principles generally project the true dynamical equations into a finite-dimensional functional spaces, which are generated by a finite number of basis functions $\{\chi_{k}\}$ such that

$$\left\langle \chi_{k} \left| \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \right| \phi \right\rangle = 0.$$ \hspace{1cm} (12)

This variational procedure is widely known as the Dirac-Frenkel principle, and not much difficulty is encountered in the ordinary practice.
2.2.2. A basic structure of Kan’s method

Kan’s theory [17] starts with the standard variational principle with a functional

$$\delta \int \left\{ \phi(\alpha) \left| \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi(\alpha) \right| dt = 0, \right.$$  \hspace{1cm} (13)

where $\alpha$ is a vector of real-valued parameters. An equation of motion naturally emerges as the Euler–Lagrange equation such that

$$\frac{\partial}{\partial \alpha} \mathcal{F} - \frac{d}{dt} \frac{\partial}{\partial \dot{\alpha}} \mathcal{F} = 0,$$

where

$$\mathcal{F} = \left\{ \phi(\alpha) \left| \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi(\alpha) \right| \right.$$

Further, noting the relation

$$\sum_{k} \left[ \frac{d\phi(\alpha)}{d\alpha_k} \right] \left[ \frac{d\phi(\alpha)}{d\alpha_j} \right] - \left[ \frac{d\phi(\alpha)}{d\alpha_k} \right] \left[ \frac{d\phi(\alpha)}{d\alpha_j} \right] \right\} \frac{d\alpha_k}{dt} = \frac{\partial}{\partial \alpha_j} \langle \phi(\alpha) | \hat{H} | \phi(\alpha) \rangle.$$  \hspace{1cm} (17)

In terms of the following matrix

$$B_{jk} = i\hbar \left\{ \frac{d\phi(\alpha)}{d\alpha_j} \left| \frac{d\phi(\alpha)}{d\alpha_k} \right| \right\} - \left\{ \frac{d\phi(\alpha)}{d\alpha_k} \right| \frac{d\phi(\alpha)}{d\alpha_j} \right\},$$

Equation (17) can be rewritten as

$$\frac{d\alpha_k}{dt} = \sum_{j} B_{jk}^{-1} \frac{\partial}{\partial \alpha_j} \langle \phi(\alpha) | \hat{H} | \phi(\alpha) \rangle.$$  \hspace{1cm} (19)

Thus the time dependent Schrödinger equation has been transformed into a set of simultaneous ordinary differential equations over the space of variational parameters [17].

A serious problem involved in equation (19) is that the matrix $B$ there, equation (18), can be singular and accordingly $B^{-1}$ in the vicinity of the singular points will behave erroneous. It is expected that the number of those singular points will increase as the number of variational parameters. Also, the matrix $B$ becomes null whenever the trial function happens to be real-valued. Kan himself exploited a method to avoid such singularities [17], but the procedure proposed seems to be too complicated to carry out at each step of numerical integration of the coupled ordinary differential equations. From the view point of numerical analysis, such singularity can be formally removed by means of the methods like singular decomposition at each point of divergence. Yet two kinds of singularities are expected; one is accidental, which may be augmented by interpolation and/or extrapolation techniques, and the other is more systematically caused, which can take place simultaneously in multiple parameter coordinates depending on physical situations under study. It is not nice anyway for any initial value problem to encounter singularities on the way of tracking its trajectories, since information prepared in the initial conditions may be lost and the accuracy can be sacrificed to a large extent.

In his study Kan came to a conclusion that there is no Legendre transformation that allows $d\alpha_k/dt$ to be treated as independent variables as momenta in classical mechanics. This is because the right hand side of equation (19) does not contain momentum-like variables like $d\alpha_k/dt$ [17].

2.2.3. Kan’s method from the view point of the Dirac-Frenkel

In the linear equation of equation (12) one may insert $\phi(\alpha)$ as a trial function such that

$$\sum_{j} \frac{d\alpha_j}{dt} \left\{ \chi_k \left| \frac{d\phi(\alpha)}{d\alpha_j} \right| \right\} = \frac{1}{i\hbar} \langle \chi_k | \hat{H} | \phi(\alpha) \rangle,$$

for an arbitrary set of $\{\chi_k\}$. Note that the set $\{\chi_k\}$ may include even those functions that are not used to expand the trial function. Then assuming that the following matrix
\[ A_{ij} = \left\langle \chi_k \left| \frac{\partial \phi(\alpha)}{\partial \alpha_j} \right. \rightangle \]  

is a square nonsingular one, we ‘formally’ have

\[ \frac{d\alpha_k / dt}{i\hbar} = A^{-1} \left\langle \chi_k | \hat{H} | \phi(\alpha) \right. \rangle. \]

\[ A \text{ turns out to be a unit matrix when only the linear parameters are adopted as in equation (10) and those basis functions are all orthonormal. This linearization method looks very straightforward. However, equation (20) works as a good approximation only when the parameter set \{\alpha_j\} is large enough, at a risk of singularity of } A, \]

As suggested by Broeckhove et al, we may choose the following particular basis functions

\[ \chi_k = \frac{\partial \phi(\alpha)}{\partial \alpha_k} \]

and impose the conditions in equation (12) (without knowing the variational principle behind)

\[ \left\{ \frac{\partial \phi(\alpha)}{\partial \alpha_k} \right| \left( \frac{i\hbar}{\lambda} \frac{\partial}{\partial t} - \hat{H} \right) \left| \phi(\alpha) \right. \rangle = 0. \]

We then have

\[ i\hbar \sum_j \frac{d\alpha_j}{dt} \left\langle \frac{\partial \phi(\alpha)}{\partial \alpha_j} \left| \frac{\partial \phi(\alpha)}{\partial \alpha_k} \right. \right. \right. \rangle = \left\langle \frac{\partial \phi(\alpha)}{\partial \alpha_k} | \hat{H} | \frac{\partial \phi(\alpha)}{\partial \alpha_k} \right. \rangle. \]

Further, take the complex conjugate

\[ -i\hbar \sum_j \frac{d\alpha_j}{dt} \left\langle \frac{\partial \phi(\alpha)}{\partial \alpha_j} \left| \frac{\partial \phi(\alpha)}{\partial \alpha_k} \right. \right. \right. \rangle = \left\langle \phi(\alpha) | \hat{H} | \frac{\partial \phi(\alpha)}{\partial \alpha_k} \right. \rangle, \]

assuming the parameters \( \alpha_j \) are all real as adopted in the Kan theory [17]. Summing up these two equalities we see

\[ i\hbar \sum_j \left\langle \frac{\partial \phi(\alpha)}{\partial \alpha_k} \left| \frac{\partial \phi(\alpha)}{\partial \alpha_j} \right. \right. \right. \rangle - \left\langle \frac{\partial \phi(\alpha)}{\partial \alpha_j} \left| \frac{\partial \phi(\alpha)}{\partial \alpha_k} \right. \right. \right. \rangle \frac{d\alpha_j}{dt} = \left\langle \frac{\partial \phi(\alpha)}{\partial \alpha_k} | \hat{H} | \phi(\alpha) \right. \rangle, \]

which is exactly the same as Kan’s equation (17). Thus, we may say that the Kan method is a linearization approximation in equation (13) with respect to the nonlinear parameters, and the matrix inversion is unavoidable in this context.

**2.3. McLachlan method**

Far before the Kan theory, McLachlan had proposed a method [16] to extract the solution of the time-dependent Schrödinger equation applying a minimum principle to

\[ \left\langle \phi \left| \left( \frac{i\hbar}{\lambda} \frac{\partial}{\partial t} - \hat{H} \right)^2 \phi \right. \rangle \right. \]

An impression may suggest that this minimization procedure should give more accurate results than the stationary procedure of Kan’s method and heavier numerical burden is demanded as a consequence. Broeckhove et al [19] have analyzed the interrelationship between the two variational method and found a remarkable fact that these two are essentially equivalent to each other, if the variational parameters have the pairwise complementary forms such that

\[ (u, v) = \begin{pmatrix} u_1 & \cdots & u_k & \cdots \\ v_1 & \cdots & v_k & \cdots \end{pmatrix}, \]

where they are all real-valued and satisfy individually

\[ i\frac{\partial \phi}{\partial u_j} = \frac{\partial \phi}{\partial v_j} \text{ for all } j. \]

Thus \((u_0, v)\) is essentially the real and imaginary parts of a complex number. In this regard, a general TDVP in the coherent representation of Gaussian basis developed by Shalashilin and Burghardt is also important [23].
3. Dual least action principle in parameter space

In what follows we consider trial wavefunctions in a form of \( \phi(u, v) \), in which real-valued vectors \( u \) and \( v \) are supposed to have pairwise components \( (u_i, v_i) \) as in equation (29). We here consider only time-independent Hamiltonian, yet most of the resultant dynamical equations of motion are valid even for time-dependent Hamiltonians.

3.1. Variational principle for energy conservation

It is widely known that the Hamilton-like canonical equations of motion for energy expectation value work to determine specific class of variational parameters. Take a simple coherent type trial function as an example

\[
\phi(q, t) = N(t) \exp\left(-\alpha(q - q_0(t))^2 + \frac{i}{\hbar} p_0(t)(q - q_0(t))\right),
\]

with \( \alpha \) being frozen. Putting \( u = q_0 \) and \( v = p_0 \) we can track them in time be means of the following equations of motion

\[
\frac{du}{dt} = \frac{\partial(\phi|\hat{H}|\phi)}{\partial v}
\]

and

\[
\frac{dv}{dt} = -\frac{\partial(\phi|\hat{H}|\phi)}{\partial u}.
\]

Obviously this dynamics is far more manageable than the Kan dynamics. Along the flow lines \( (u(t), v(t)) \) thus determined, the energy conservation is readily ensured by the relation

\[
\frac{d}{dt} \langle \phi(u, v)|\hat{H}|\phi(u, v) \rangle = 0.
\]

An advantage of this simple method is that quantum effects such as the zero-point energy along the path are partly taken into account, and yet their resultant paths can be similar to those of the classical counterpart. The question is which class of parameters can be determined only by means of equations (32) and (33). We will be back to this issue later in the next section.

A variational functional that conserves the energy can be readily made up in analogy to the classical least action principle of equation (5), which is simply written as

\[
S_H = \int_C (v \cdot \dot{u} - (\phi|\hat{H}|\phi)) dt,
\]

where \( \alpha \) indicates arbitrary time interval under study. In what follows \( \phi \) is always assumed to be normalized and therefore the normalization constant is subject to the variational operation. The variation of \( S_H \) gives

\[
\delta S_H = \int_C \left(\delta u \cdot \dot{u} + u \cdot \delta v - \frac{\partial(\phi|\hat{H}|\phi)}{\partial u} \cdot \delta u - \frac{\partial(\phi|\hat{H}|\phi)}{\partial v} \cdot \delta v\right) dt
\]

\[= \int_C \left(\frac{dv}{dt} - \frac{\partial(\phi|\hat{H}|\phi)}{\partial u} \cdot \delta u + \left(\frac{du}{dt} - \frac{\partial(\phi|\hat{H}|\phi)}{\partial v}\right) \cdot \delta v\right) dt
\]

\[= (v \cdot \delta u)_{\text{rad}}^2 + \int_C \left(\frac{dv}{dt} - \frac{\partial(\phi|\hat{H}|\phi)}{\partial u} \cdot \delta u + \left(\frac{du}{dt} - \frac{\partial(\phi|\hat{H}|\phi)}{\partial v}\right) \cdot \delta v\right) dt
\]

under the fixed boundary condition

\[= (v \cdot \delta u)_{\text{rad}}^2 = 0.
\]

Since both \( \delta u \) and \( \delta v \) in equation (36) are individually arbitrary, \( \delta S_H = 0 \) requires equations (32) and (33) to identically hold. Note that the Maupertuis reduced action is seen as \( v \cdot \dot{u} \) in \( S_H \).

Any trajectories \( (u(t), v(t)) \) in parameter space should satisfy the energy conservation. Yet, it is obvious that the energy conservation alone is not enough to determine correct trajectories. In other words, \( \delta S_H = 0 \) or equations (32)–(33) are insufficient. Something is missing.

3.2. Dual least action principle

The missing factor is readily identified in the full variational principle

\[
\delta \int_C \left(\phi(u, v) \left| i\hbar \frac{\partial}{\partial t} - \hat{H} \right| \phi(u, v) \right) dt = 0,
\]
by subtracting $\delta S_{H}$ from it as

$$\delta \int_C \left( \phi \left( i \hbar \frac{\partial}{\partial t} \phi - \hat{H} \phi \right) \right) dt - \delta \int_C \left( v \cdot \dot{u} - \left( \phi | \hat{H} | \phi \right) \right) dt = - \delta \int_C \left( \phi \left( i \hbar \frac{\partial}{\partial t} \left( \phi | \phi \right) \right) dt. \right. \tag{39}$$

This subtraction is mathematically valid since the variation is a linear operation with respect to variational functionals. Thus we find and define a variational functional

$$S_W(u, v) = \int_C \left( v \cdot \dot{u} - \left( \phi | i \hbar \frac{\partial}{\partial t} \phi \right) \right) dt = \int_C \left( v \cdot \dot{u} - \left( \phi | \hat{H} | \phi \right) \right) dt. \tag{40}$$

Since $S_W$ is the counterpart of $S_{H}$, equation (38) is equivalently rewritten as

$$\delta S_{H}(u, v) - \delta S_W(u, v) = 0. \tag{41}$$

As far as the exact solutions are concerned, the condition of equation (41) along with $\delta S_{H}(u, v) = 0$ demands

$$\delta S_W(u, v) = 0,$$  \tag{42}

which is responsible for the Schrödinger 'wave dynamics'. Note, however, that $\delta S_{H}(u, v) = 0$ and $\delta S_W(u, v) = 0$ are never independent from each other. Only the exact $\phi(u, v)/s$ are supposed to satisfy both of these variational conditions simultaneously. We thus need to study the simultaneous variational principles

$$\begin{cases} \delta S_{H}(u(t), v(t)) - \delta S_W(u(t), v(t)) = 0 \\ \delta S_{H}(u(t), v(t)) = 0 \\ \delta S_W(u(t), v(t)) = 0 \end{cases} \tag{43}$$

or more simply

$$\delta S_{H}(u(t), v(t)) = \delta S_W(u(t), v(t)) = 0,$$ \tag{44}

where $(u(t), v(t))$ in $S_{H}$ and $S_W$ should be common. Equation (43) or (44) is referred to as a dual least action principle.

The condition in equation (43) should be formally stronger than the total variational condition of equation (39) is, since the latter can hold under a weaker situation in which the deviation from zero in $\delta S_W$ and that in $\delta S_{H}$ happen to cancel each other. On the other hand, it is hard to anticipate that the errors arising from $\delta S_{H} = 0$ and $\delta S_W = 0$ are compensated well. Indeed, as we will see later, the physical and mathematical natures of $\delta S_{H}$ and $\delta S_W$ are so much different from each other that such systematic cancellation of errors is hardly expected to happen.

An obvious reason why the functional $S_W$ appears to be necessary is because $S_{H}$ of equation (35) alone cannot reflect the Schrödinger dynamics. For instance, in order to distinguish the dynamics arising from

$$i \hbar \frac{\partial}{\partial t} \phi = \hat{H} \phi \tag{45}$$

or hypothetical (or Klein–Gordon) dynamics

$$\frac{\partial^2}{\partial t^2} \phi = \hat{H} \phi \tag{46}$$

the explicit functional form of $S_W$ is definitely needed. Hence the condition $\delta S_W = 0$ identifies the way of propagation of the 'waves', while $\delta S_{H} = 0$ is mainly responsible for energetics of 'trajectory motion' of the wavepacket.

Just as the $\delta S_{H} = 0$ has given equations (32) and (33), $\delta S_W = 0$ formally brings about

$$\frac{du}{dt} = i \hbar \frac{\partial}{\partial v} \langle \phi | \dot{\phi} \rangle \tag{47}$$

and

$$\frac{dv}{dt} = -i \hbar \frac{\partial}{\partial u} \langle \phi | \dot{\phi} \rangle, \tag{48}$$

which represents a 'flow conservation' (see below) along the path

$$\frac{d}{dt} \langle \phi | \dot{\phi} \rangle = \frac{dv}{dt} \cdot \frac{\partial \langle \phi | \dot{\phi} \rangle}{\partial v} + \frac{du}{dt} \cdot \frac{\partial \langle \phi | \dot{\phi} \rangle}{\partial u} = 0. \tag{49}$$

In this conjunction, we note that $v \cdot \dot{u}$ in this stage is no longer regarded as a factor to induce the Legendre transformation but has been introduced to find the stationary paths and invariances in the parameter spaces in analogy to classical mechanics. Also, recalling the 2-form
\[
\int \mathbf{v} \cdot d\mathbf{u} = \int d\mathbf{v} \wedge d\mathbf{u} = - \int d\mathbf{u} \wedge d\mathbf{v} = - \int \mathbf{u} \cdot d\mathbf{v},
\]

we identify \( \mathbf{v} \cdot d\mathbf{u} \) in this context as a quantity related to an absolute invariance in the parameter space [28], which will be discussed in subsection 3.5.

Once again we stress that the set equations (32)–(33) and that of equations (47)–(48) are not to be integrated separately. They are supposed to represent a tightly coupled mechanics of Hamiltonian dynamics and wave flow dynamics as a one unit.

### 3.3. Quantum flux for the wave dynamics in parameter space

We here survey the physical meaning of \( \delta S_W = 0 \), which highlights the characteristics of the Schrödinger wave dynamics. The study about how to treat equation (43) in practical approximations will be resumed in section 3.4.

#### 3.3.1. Quantum flux in parameter space

We first write in \( S_W \)

\[
\imath \hbar \langle \phi | \dot{\phi} \rangle = \frac{i\hbar}{2} (\langle \phi | \dot{\phi} \rangle - \langle \phi | \phi \rangle),
\]

which is real-valued, and rewrite the right hand side as

\[
\langle \phi | \dot{\phi} \rangle - \langle \phi | \phi \rangle = \frac{d\mathbf{u}}{dt} \cdot \int \left( \phi^* \frac{\partial \phi}{\partial \mathbf{u}} - \phi \frac{\partial \phi^*}{\partial \mathbf{u}} \right) d\mathbf{q}
\]

\[
+ \frac{d\mathbf{v}}{dt} \cdot \int \left( \phi^* \frac{\partial \phi}{\partial \mathbf{v}} - \phi \frac{\partial \phi^*}{\partial \mathbf{v}} \right) d\mathbf{q}.
\]

Here

\[
\int \left( \phi^* \frac{\partial \phi}{\partial \mathbf{u}} - \phi \frac{\partial \phi^*}{\partial \mathbf{u}} \right) d\mathbf{q}.
\]

for instance, corresponds to the gradient of the field of fluid in \( \mathbf{u} \)-direction. To be more precise, let us recall the definition of quantum mechanical flux (current of probability density) [30], which is defined as

\[
\mathbf{j}(\mathbf{q}) = \frac{i\hbar}{2m} (\phi^* \nabla \phi - \phi \nabla \phi^*),
\]

with the mass \( m = 1 \). By analogy, we may define fluxes in the parameter space such that

\[
\mathbf{j}_u = \frac{i\hbar}{2} \int \left( \phi^* \frac{\partial \phi}{\partial \mathbf{u}} - \phi \frac{\partial \phi^*}{\partial \mathbf{u}} \right) d\mathbf{q} = - \hbar \imath \text{Im} \left[ \phi \frac{\partial \phi}{\partial \mathbf{u}} \right],
\]

which is the probability current in the \( \mathbf{u} \) direction, and likewise the flux in the \( \mathbf{v} \)-direction is

\[
\mathbf{j}_v = \frac{i\hbar}{2} \int \left( \phi^* \frac{\partial \phi}{\partial \mathbf{v}} - \phi \frac{\partial \phi^*}{\partial \mathbf{v}} \right) d\mathbf{q} = - \hbar \imath \text{Im} \left[ \phi \frac{\partial \phi}{\partial \mathbf{v}} \right].
\]

And therefore we have

\[
\imath \hbar \langle \phi | \dot{\phi} \rangle = \frac{d\mathbf{u}}{dt} \cdot \mathbf{j}_u + \frac{d\mathbf{v}}{dt} \cdot \mathbf{j}_v,
\]

which gives an alternative interpretation of \( \langle \phi | \dot{\phi} \rangle \) in terms of the flow in the parameter space.

Let us briefly detour to a complex-valued flux emerging from \( \mathbf{j}_u \) and \( \mathbf{j}_v \). Define complex coordinates as Broeckhove et al. did [19] such that

\[
\mathbf{z} = \mathbf{u} + i\mathbf{v} \quad \text{and} \quad \mathbf{z}^* = \mathbf{u} - i\mathbf{v}.
\]

Then we have

\[
\mathbf{j}_z = \frac{1}{2} \left( \mathbf{j}_u - i \times \mathbf{j}_v \right)
\]

and

\[
\mathbf{j}_z^* = \frac{1}{2} \left( \mathbf{j}_u + i \times \mathbf{j}_v \right),
\]

which highlight the role of the pairwise complementary parameters \( \mathbf{u} \) and \( \mathbf{v} \) (see also [23]).
Back to equations (47)–(48), they are thus rewritten, respectively, as
\[
\frac{du}{dt} = i\hbar \frac{\partial (\phi | \dot{\phi})}{\partial v} = \frac{\partial}{\partial v} \left( \frac{du}{dt} \cdot j_u + \frac{dv}{dt} \cdot j_v \right)
\]  
(62)

and
\[
\frac{dv}{dt} = -i\hbar \frac{\partial (\phi | \dot{\phi})}{\partial u} = -\frac{\partial}{\partial u} \left( \frac{du}{dt} \cdot j_u + \frac{dv}{dt} \cdot j_v \right).
\]  
(63)

It is interesting to see the nonlinear nature of the dynamics manifest itself in the right hand sides of equations (62) and (63), where \( \frac{du}{dt} \) and \( \frac{dv}{dt} \), respectively, appear. This kind of nonlinearity is seen rather frequently in fluid dynamics.

3.3.2. Simple yet exceptional example of the flux
For a later purpose, we here show an example of the flux arising from the so-called coherent state wavepacket
\[
\phi(q, t) = N \exp \left( -\alpha(t) + i\beta(t)(q - q_0(t)) \right) \times \exp \left( i \frac{p_0(t)(q - q_0(t))}{\hbar} \right),
\]  
(64)

which is frequently used as an expansion basis [23]. The parameters \( q_0 \) and \( p_0 \) are often treated as dynamically conjugate parameters. Taking \( q_0 \) and \( p_0 \) as one of the \( u \) and \( v \) parameters, respectively, we readily see the following relation
\[
j_{u_0} = p_0,
\]  
(65)

which seems natural and is indeed consistent with the quantum momentum operator \( \hat{p} = \frac{\hbar}{i} \nabla \) in that
\[
p_0 = -\frac{\hbar}{i} \left\langle \phi \left| \frac{\partial \phi}{\partial q_0} \right\rangle \right.,
\]  
(66)

where the minus sign arises from \( -q_0(t) \) in the representation of equation (64). As for the \( j_{p_0} \), on the other hand, we see
\[
j_{p_0} = -\hbar \text{Im} \left\langle \phi \left| \frac{\partial \phi}{\partial p_0} \right\rangle \right. = 0.
\]  
(67)

This trivial-looking example will play an illustrative role later in the argument of classification of parameters.

3.3.3. Equations of motion for the wave dynamics

Equations (62)–(63) are nonlinear as stated above. In addition, \( i\hbar \langle \phi | \dot{\phi} \rangle \) contains no information about what kind of driving forces are working on \( \phi \). To resolve these issues at a time, we implant equations (32)–(33) as \( \frac{du}{dt} \) and \( \frac{dv}{dt} \) in the right hand sides of equations (62)–(63), respectively, such that
\[
\frac{du}{dt} = \frac{\partial}{\partial v} \left( \frac{\partial (\phi | \dot{\phi})}{\partial \phi} \cdot j_u - \frac{\partial (\phi | \dot{\phi})}{\partial \phi} \cdot j_v \right)
\]  
(68)

and
\[
\frac{dv}{dt} = -\frac{\partial}{\partial u} \left( \frac{\partial (\phi | \dot{\phi})}{\partial \phi} \cdot j_u - \frac{\partial (\phi | \dot{\phi})}{\partial \phi} \cdot j_v \right).
\]  
(69)

These serve as our working equations, which should be integrated together with equations (32)–(33).

In equations (68) and (69), we see the factor
\[
\frac{\partial (\phi | \dot{\phi})}{\partial v} \cdot j_u - \frac{\partial (\phi | \dot{\phi})}{\partial u} \cdot j_v = \left( \frac{\partial (\phi | \dot{\phi})}{\partial u} \frac{\partial (\phi | \dot{\phi})}{\partial v} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} j_u \\ j_v \end{pmatrix}
\]  
(70)

which is a symplectic inner product between the Hamiltonian derivative vector and the flux vector. Hence this quantity represents a coupling between the Hamiltonian dynamics (so to say particle dynamics) and the motion of the spatial redistribution of probability density (wave dynamics). All the effects with respect to the deformation of wavefunctions manifest themselves through these couplings.

3.4. Two sets of dynamics to be tracked 'simultaneously'

3.4.1. Connecting piecewise trajectories
If our trial function \( \phi(u(t), v(t)) \) were given beforehand as an exact solution of the Schrödinger equation having a proper set of infinite number of parameters, the two dynamical equations, equations (32)–(33) from the
Hamilton dynamics and equations (62–63) (or equations (68–69)) from the wave flow dynamic, are supposed to be satisfied simultaneously, simply because they are satisfied by $i\hbar \frac{\partial}{\partial t} \phi = \hat{H} \phi$. However, our trial functions are not exact in general, and we need to treat both equations (32–33) and (62–63) as pairwise simultaneous conditions to guide $(u(t), v(t))$ toward the correct trajectories. We below consider this aspect in a little more systematic manner.

Suppose we have a short time approximate solution in equations (32–33), which is formally written as

$$\begin{align*}
\begin{bmatrix} u(t+\Delta t) \\ v(t+\Delta t) \end{bmatrix}_H &= F(t; \Delta t) \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_H, \\
\begin{bmatrix} u(t+\Delta t) \\ v(t+\Delta t) \end{bmatrix}_W &= G(t; \Delta t) \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_W.
\end{align*}
$$

(71)

and likewise from equations (62–63)

$$\begin{align*}
\begin{bmatrix} u(t+\Delta t) \\ v(t+\Delta t) \end{bmatrix}_H &= F(t; \Delta t) \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_H, \\
\begin{bmatrix} u(t+\Delta t) \\ v(t+\Delta t) \end{bmatrix}_W &= G(t; \Delta t) \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_W.
\end{align*}
$$

(72)

The suffixes $H$ and $W$ indicate the Hamilton dynamics and the wave-flow dynamics, respectively. Finite time solution of each is to be formally given as

$$\begin{align*}
\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_H &= F(t-\Delta t; \Delta t) \cdots F(\Delta t; \Delta t) F(0; \Delta t) \begin{bmatrix} u(0) \\ v(0) \end{bmatrix}, \\
\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_W &= G(t-\Delta t; \Delta t) \cdots G(\Delta t; \Delta t) G(0; \Delta t) \begin{bmatrix} u(0) \\ v(0) \end{bmatrix},
\end{align*}
$$

(73)

and

$$\begin{align*}
\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_H &= F(t-\Delta t; \Delta t) \cdots F(\Delta t; \Delta t) F(0; \Delta t) \begin{bmatrix} u(0) \\ v(0) \end{bmatrix}, \\
\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_W &= G(t-\Delta t; \Delta t) \cdots G(\Delta t; \Delta t) G(0; \Delta t) \begin{bmatrix} u(0) \\ v(0) \end{bmatrix},
\end{align*}
$$

(74)

If $\phi(u(t), v(t))$ was exact globally in the parameter space, it should hold that $F(t; \Delta t) = G(t; \Delta t)$ under the same initial conditions and

$$\begin{align*}
\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_H &= \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}_W.
\end{align*}
$$

(75)

However, in our practical approximations, these two solutions at a finite time $t$ should deviate from each other to a significant extent. Therefore we should abandon the pursuit of the exact propagation. Instead we assume that the simultaneous variational principles $\delta S_H = 0$ and $\delta S_W = 0$ are satisfied only for each very short time segments $\Delta t$. Therefore the finite time solutions are to be obtained by connecting the short-time segment solutions such that, for instance,

$$\begin{align*}
\begin{bmatrix} u(t) \\ v(t) \end{bmatrix} = \lim_{\Delta t \to 0} G(t-\Delta t/2; \Delta t/2) F(t-\Delta t; \Delta t/2) \cdots G(\Delta t/2; \Delta t/2) F(0; \Delta t/2) \begin{bmatrix} u(0) \\ v(0) \end{bmatrix}.
\end{align*}
$$

(76)

Note that there can be many variants to replace this simplest alternate products, just as in the higher-order symplectic integrators [31]. The procedure in equation (76) technically equivalent to the alternate integration of

$$\begin{align*}
\frac{du^{(1)}}{dt} &= \frac{\partial}{\partial u^{(1)}} \left\{ \phi(u^{(1)}, v^{(1)}) | \hat{H} | \phi(u^{(1)}, v^{(1)}) \right\} |_{u^{(1)=1}, v^{(1)=1}, v^{(2)=2}}, \\
\frac{dv^{(1)}}{dt} &= -\frac{\partial}{\partial v^{(1)}} \left\{ \phi(u^{(1)}, v^{(1)}) | \hat{H} | \phi(u^{(1)}, v^{(1)}) \right\} |_{u^{(2)=2}, v^{(1)=1}, v^{(2)=2}},
\end{align*}
$$

(77)

for an interval from $t$ to $t + \Delta t/2$ and next one

$$\begin{align*}
\frac{du^{(2)}}{dt} &= i\hbar \frac{\partial}{\partial u^{(2)}} \left\{ \phi(u^{(2)}, v^{(2)}) | \hat{H} | \phi(u^{(2)}, v^{(2)}) \right\} |_{u^{(1)=1}, v^{(1)=1}, v^{(2)=2}}, \\
\frac{dv^{(2)}}{dt} &= -i\hbar \frac{\partial}{\partial v^{(2)}} \left\{ \phi(u^{(2)}, v^{(2)}) | \hat{H} | \phi(u^{(2)}, v^{(2)}) \right\} |_{u^{(2)=2}, v^{(1)=1}, v^{(2)=2}},
\end{align*}
$$

(78)

for an interval from $t + \Delta t/2$ to $t + \Delta t$, where $u^{(1)} \leftarrow u^{(2)}, v^{(1)} \leftarrow v^{(2)}$, for instance, in the suffix of these equations indicate that the values of $u^{(2)}$ and $v^{(2)}$ are to be respectively inserted into $u^{(1)}$ and $v^{(1)}$ before each integration is performed for an interval $\Delta t/2$. The variational parameters $(u(t), v(t))$ thus tracked are continuous but not necessarily smooth.

### 3.4.2. On the initial conditions to be consistent between Hamilton dynamics and flow dynamics

We note that for $du/\ dt$ and $dv/\ dt$ of equations (32–33) and equations (47–48) (in place of equations (68–69) for shorter notation) to be mathematically consistent, the following condition needs to be fulfilled (either rigorously or approximately for short time intervals): A straightforward combination of equations (34) and (49) gives rise to
\[
\left( \frac{\partial}{\partial t} \langle \hat{H} \mid \phi \rangle / \partial u \quad \frac{\partial}{\partial t} \langle \hat{H} \mid \phi \rangle / \partial v \right) \frac{du}{dt} \frac{dv}{dt} = 0.
\]

And, in order for equation (79) to give nontrivial solutions for the vector \((du/dt, dv/dt)\), the relevant determinant should vanish, that is,
\[
\left| \begin{array}{cc}
\frac{\partial}{\partial t} \langle \hat{H} \mid \phi \rangle / \partial u & \frac{\partial}{\partial t} \langle \hat{H} \mid \phi \rangle / \partial v \\
\frac{\partial}{\partial t} \langle \phi \mid \hat{\phi} \rangle / \partial u & \frac{\partial}{\partial t} \langle \phi \mid \hat{\phi} \rangle / \partial v
\end{array} \right| = 0.
\]

If, on the other hand, either the functional form of a trial function or the parameter setting in it, or both, is not appropriate enough to approximate the Schrödinger dynamics \(i\hbar \frac{\partial}{\partial t} \phi(u, v) = 0\), the above condition is not satisfied and consequently the ordinary differential equations (ODEs) cannot be integrated.

Likewise, we need to pay attention to the choice of initial conditions \((u(0), v(0))\). Practically, we impose the conditions
\[
\text{det} \left| \begin{array}{cc}
\frac{\partial}{\partial t} \langle \hat{H} \mid \phi \rangle / \partial u_{i} & \frac{\partial}{\partial t} \langle \hat{H} \mid \phi \rangle / \partial v_{i} \\
\frac{\partial}{\partial t} \langle \phi \mid \hat{\phi} \rangle / \partial u_{i} & \frac{\partial}{\partial t} \langle \phi \mid \hat{\phi} \rangle / \partial v_{i}
\end{array} \right| = 0
\]
on each pair of the initial components \((u_{i}(0), v_{i}(0))\), with consistency with the conditions for other parameters. For instance, we first give \(u_{i}(0)\) at our convenience to start the dynamics, and find \(v_{i}(0)\) as a solution of equation (81). Then both the Hamilton dynamics and wave-flow dynamics in equation (76) will be launched consistently. If, on the other hand, such a pair of \((u_{i}(0), v_{i}(0))\) is not found, those choice of functional form of parameters and/or initial conditions are judged to be ill.

3.5. Integral invariance for the quantum reduced action in parameter space
Before closing this section, we discuss invariant properties of the reduced action \(v \cdot \dot{u}\). Under an assumption that both of the two sets of equations (32)–(33) and equations (47)–(48) are simultaneously satisfied, it is straightforward to see that the divergence of the vector field \((du/dt, dv/dt)\) be zero [28], that is,
\[
\frac{\partial}{\partial u} \cdot \frac{du}{dt} + \frac{\partial}{\partial v} \cdot \frac{dv}{dt} = 0,
\]
which in turn ensures that \((u(t), v(t))\) forms an incompressible flow in parameter space as in the classical Liouville theorem. Then we may take a continuous closed curve in this parameter space, say \(\partial \Omega\), so as to be transversal to the flow of \((u(t), v(t))\). Then due to the Stokes theorem, the population passing across the area \(\Omega\), which is encircled by its closed boundary \(\partial \Omega\), is given as
\[
\int_{\partial \Omega} v \cdot du = \int_{\Omega} dv \wedge du.
\]
This quantity is conserved along \((u(t), v(t))\) as long as the flow is unique and incompressible [28]. We thus can return to the variational functionals \(S_{\mu}\) of equation (35) and \(S_{\nu}\) of equation (40) with this reasoning of the dynamics of the reduced action.

4. Conditions for the energy conservation alone to give correct parameter paths
It is obvious that the Hamilton dynamics alone does not generally lead to the correct Schrödinger dynamics. Nevertheless there are exceptional cases in which equations (32)–(33) alone can reproduce correct parameter paths with no need of the set of equations (47)–(48). Since this observation is widely accepted to be valid without theoretical account, we here study this aspect.

4.1. Variational parameters not to require the wave-flow specification
We resume the standard variational principle, equation (38), with respect to \(\phi(u, v)\). If it happens to hold, for instance,
\[
-\jmath_{u} = v
\]
and
\[
-\jmath_{v} = 0,
\]
we observe \(S_{\nu}\) be identically nullified because
\[
S_{\nu} = \int \left( v \cdot \dot{u} - \left[ \phi(u, v) \left| i\hbar \frac{\partial}{\partial t} \phi(u, v) \right| \right] \right) dt = \int \left( v \cdot \dot{u} - i\hbar \phi \cdot \left( \frac{\partial \phi}{\partial u} - \frac{\partial \phi}{\partial v} \cdot \phi \right) \right) dt = 0,
\]
(see equations (56) and (57) for the definition of the fluxes). These pairs of parameters that automatically (due to the mathematical construction) satisfy equation (86) are referred to as dynamical pair. Therefore the entire variational functional is reduced to

$$\delta \int \left\{ \phi (u, v) \left( i \hbar \frac{\partial}{\partial t} - \hat{H} \right) \right\} \phi (u, v) \, dt = \delta \int (v \cdot \dot{u} - \langle \phi (u, v) | \hat{H} | \phi (u, v) \rangle) \, dt = 0, \tag{87}$$

which is exactly the same as $\delta S_H = 0$ of equation (35). Thus the Maupertuis reduced action is directly retrieved for the dynamical pairs, and we are left only with the ODE of the type of the Hamilton canonical equations, equations (32)–(33).

Incidentally, we do not have to impose the initial condition equation (81) on the dynamical pairs, since both equations (47)–(48) are already satisfied.

We stress again that for those parameters that do not satisfy the conditions like equations (84)–(85), not only $S_H$ but $S_W$ is definitely subject to the Maupertuis–Hamilton variational principle to determine the flow of quantum wave.

4.1.1. Example 1: Coherent state wavepackets

As an example of the dynamical pair, we recall the pair of variables $(u, v) = (q_0, p_0)$ in equation (64), for which the fluxes satisfy equations (65) and (67)

$$i_j = \hbar \left\langle \frac{\partial \phi}{\partial u} \right\rangle = -\hbar \text{Im} \left\langle \phi \frac{\partial \phi}{\partial u} \right\rangle = v \tag{88}$$

and

$$i_j = -\hbar \text{Im} \left\langle \phi \frac{\partial \phi}{\partial v} \right\rangle = 0, \tag{89}$$

respectively. This is exactly the case in which the conditions equations (84)–(85) are satisfied.

Incidentally, let us further consider the term $\partial \langle \phi | \hat{\phi} \rangle / \partial \nu$ in equation (49), which is

$$\frac{\partial \langle \phi | \hat{\phi} \rangle}{\partial \nu} = \frac{\partial}{\partial \nu} \left( \frac{du}{dt} \hbar + \frac{dv}{dt} j_v \right) = \frac{\partial}{\partial \nu} \left( \frac{du}{dt} j_u \right) = \frac{du}{dt}, \tag{90}$$

where equations (88) and (89) have been used. Bringing this result back into equation (49), we have

$$\frac{d}{dt} \langle \phi | \hat{\phi} \rangle = \frac{du}{dt} \frac{\partial \langle \phi | \hat{\phi} \rangle}{\partial u} + \frac{dv}{dt} \frac{du}{dt} = 0,$$

leading to

$$\frac{dv}{dt} = -\frac{\partial \langle \phi | \hat{\phi} \rangle}{\partial u}. \tag{91}$$

Thus it turns out that equation (90) and (91) give automatically a result expected from $\delta S_W = 0$.

The identity of equation (89) is satisfied by the trial function of equation (64), because it is a symmetric Gaussian. If it is geometrically skewed as

$$\phi (q, t) = N (1 + c (q - q_0 (t))) \exp (-\alpha (t) (q - q_0 (t))^2) \times \exp \left( i \hbar p_0 (t) (q - q_0 (t)) \right), \tag{92}$$

$j_v$ in equation (89) is no longer zero, and hence $(q_0, p_0)$ is no longer a dynamical pair either. To determine these parameters we need the help of $\delta S_W = 0$. For the same reason, $(q_{01} (t), p_{01} (t))$ and $(q_{02} (t), p_{02} (t))$ in the following linear combination of one-particle one-dimensional Gaussians

$$\phi (q, t) = N \sum_{j > 2} c_j (t) \exp \left( -\alpha_j (t) (q - q_{0j} (t))^2 + i \hbar p_{0j} (t) (q - q_{0j} (t)) \right) \tag{93}$$

can lose the property of the dynamical pair as soon as the two wavepackets begin to penetrate into a zone where they mutually interfere. In this area, these classical-like parameters are responsible not only for the transport of each Gaussian but for the shape deformation of the total wavefunction $\phi (q, t)$. In such a higher quantum situation, the condition $\delta S_H = 0$ is not sufficient.

4.1.2. Example 2: Meyer–Miller transformation

Meyer and Miller proposed a quite interesting way to transform the complex linear parameters in equation (10) to ‘action-angle variables’ in such a way that
in order to treat all the quantum and classical degrees of freedom in a consistent way \[32\]. The variables thus classicalized are to be determined by the Hamilton-like equations of motion

\[
\frac{d\theta_k}{dt} = \frac{\partial \langle \phi | \hat{H} | \phi \rangle}{\partial \theta_k},
\]

and

\[
\frac{dn_k}{dt} = -\frac{\partial \langle \phi | \hat{H} | \phi \rangle}{\partial n_k},
\]

in stead of the Dirac-Frenkel variational principle equation (11). This is justified since \((\theta_k, n_k)\) forms a dynamical pair, because the flux in the \(n_k\) direction is exactly zero as

\[
\dot{j}_n = -\hbar \text{ Im} \left\{ \phi \left| \frac{\partial \phi}{\partial n_k} \right| \right\} = -\frac{\hbar}{2} \text{ Im} n_k^{1/2} = 0,
\]

provided that the basis functions in equation (10) are mutually orthogonal. Also, we have

\[
\dot{j}_n = -\hbar \text{ Im} \left\{ \phi \left| \frac{\partial \phi}{\partial \theta_k} \right| \right\} = -2\pi \hbar n_k.
\]

(We do not need to consider the normalization condition here, since \(C_k(t)\) are linear parameters, although the conclusion is the same anyway, even if normalization is made.) Here again there is no need to consider the variation with respect to \(S_W\). Note that this argument does not hold for nonorthogonal basis functions.

4.2. Role of symmetry

A trivial example of \((u, v)\) that satisfies equation (49) is

\[
\text{both } \frac{\partial \langle \phi | \dot{\phi} \rangle}{\partial u} = 0 \quad \text{and} \quad \frac{\partial \langle \phi | \dot{\phi} \rangle}{\partial v} = 0,
\]

or more simply \(\dot{u} = 0\) and \(\dot{v} = 0\). Then

\[
\text{both } \frac{d}{dt} \langle \phi | \dot{\phi} \rangle = 0 \quad \text{and} \quad \delta S_W = 0
\]

are automatically satisfied. These parameters are essentially constant (fixed in time).

Another simple yet nontrivial example is a case where the parameter pairs are related to the constant of motion just as in the classical Noether theorem \[27\]. Suppose we have a ‘continuous’ symmetry in the parameter space in \(u^0\)-direction, which is related to, for instance, spatial translation, rotation, time translation, and so on. Assume that it holds that

\[
\langle \phi(u - \Delta u^0, v) | \hat{H} | \phi(u - \Delta u^0, v) \rangle = \langle \phi(u, v) | \hat{H} | \phi(u, v) \rangle.
\]

Then it follows that

\[
\left( \left\langle \frac{\partial}{\partial u^0} \phi(u, v) \left| \phi(u, v) \right\rangle + \left\langle \phi(u, v) \left| \frac{\partial}{\partial u^0} \phi(u, v) \right\rangle \right\} = 0,\right.
\]

and one can find a constant flux \(j_{u^0}\) with respect to the \(u^0\)-variable as

\[
\dot{j}_{u^0} = -\hbar \text{ Im} \left\{ \phi \left| \frac{\partial \phi}{\partial u^0} \right| \right\},
\]

where \(\langle \phi | \partial \phi / \partial u^0 \rangle\) is pure imaginary. Then we may define \(v_0\) as a partner of the parameter \(u^0\) such that

\[
v^0 = j_{u^0} \times \text{ constant}.
\]

Hence the dynamics on the parameter set \((u^0, v^0)\) is so determined. On the other hand,

\[
\dot{j}_{v^0} = -\hbar \text{ Im} \left\{ \phi \left| \frac{\partial \phi}{\partial v^0} \right| \right\}
\]

is not zero, but this time we have

\[
v^0 = 0,
\]

and therefore equation (86) can be readily realized by rescaling \(u^0\) and \(v^0\).

There can exist other situations in which \(\delta S_W = 0\) is not demanded.
5. Concluding remarks

We have studied the time-dependent variational principle in such a way to split the variational functional

\[
\int \left\{ \phi \left| \frac{\partial}{\partial t} \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi \right| \right\} dt
\]

(106)

into \( S_H \) (equation (35)) and \( S_W \) (equation (40)), in both of which the Maupertuis reduced action in the dynamical parameter space is retrieved. A dual variational principle of the form of \( \delta S_H = \delta S_W = 0 \) or equation (43) has been formulated. For approximate wavefunctions we integrate alternately two sets of coupled Hamilton-like equations of motion, equations (77) and (78), along with good choice of the initial conditions, to seek for good paths in the parameter space.

The requirement emerging from the wave-flow dynamics through \( S_W \) represents an essential factor to reproduce the genuine Schrödinger dynamics. This dynamics is represented in terms of the quantum flux in parameter space, and their properties are critically important in classification of the nature of the parameters. As an important example, we have shown that there are classes of parameter setting that make \( \delta S_H = 0 \) automatically. For these parameters, only the Hamilton-like canonical equations of motion emerging from \( \delta S_H = 0 \) are sufficient to reproduce the correct parameter trajectories, as shown in equation (87). This aspect is relevant to the quantum–classical correspondence.

We stress again that the present variational principle does not require matrix inversion at each step of the time-integration of the relevant ODEs, equations (77)–(78) with equations (68)–(69), and is simple and free of singularity. Yet, it is hard to anticipate that the present method improves the numerical accuracy of the other standard TDVP such as the Kan’s when no singularity happens in the latter. This is because the accuracy level of them are generally limited within a range that is determined by the conditions

\[
\left. \left\{ \phi(u, v) \left| \frac{\partial}{\partial t} \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi(u, v) \right| \right\} \right|_{u=u(t), v=v(t)} = 0,
\]

(107)

\[
\left. \frac{\partial}{\partial u} \left\{ \phi(u, v) \left| \frac{\partial}{\partial t} \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi(u, v) \right| \right\} \right|_{u=u(t), v=v(t)} = 0
\]

(108)

and

\[
\left. \frac{\partial}{\partial v} \left\{ \phi(u, v) \left| \frac{\partial}{\partial t} \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi(u, v) \right| \right\} \right|_{u=u(t), v=v(t)} = 0.
\]

(109)

Equations (108) and (109) specify the geometrical structure of \( \left\{ \phi(u, v) \left| \frac{\partial}{\partial t} \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi(u, v) \right| \right\} \) nearby the paths \((u(t), v(t))\) in \((u, v)\)-space. Of course, the above conditions equations (107)–(109) are not necessarily equivalent to the full Schrödinger equation \( \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi = 0 \) itself.

The present dual least action principle had started from the Schrödinger equation and came to a variational method in the end. It would be instructive to invert this order: We ‘assume’ the set of two coupled Maupertuis-Hamilton dynamics

\[
\delta \int (v \cdot \ddot{u} - \langle \phi | \hat{H} | \phi \rangle) dt = 0
\]

(110)

and

\[
\delta \int \left( v \cdot \dot{u} - \left\{ \phi \left| \frac{\partial}{\partial t} \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi \right| \right\} \right) dt = 0
\]

(111)

to exist at the very beginning. Equation (110) corresponds to the classical Hamilton least action principle, while the latter is responsible for the wave-flow dynamics. The conservation laws emerge not only for energy but for the probability current. Thus they altogether reflect the wave-particle duality. Next, one may eliminate

\[
\delta \int v \cdot \ddot{u} dt
\]

(112)

from equations (110)–(111) and combine them into a single piece as

\[
\delta \int \left\{ \phi \left| \frac{\partial}{\partial t} \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \phi \right| \right\} dt = 0.
\]

(113)
Furthermore, the Dirac-Frenkel variational principle recovers the Schrödinger equation

$$\left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) |\phi\rangle = 0,$$

(114)

if $\phi$ can be linearly expanded in complete basis functions. Of course we now know Schrödinger ‘miraculously’ unified the wave-particle nature into a single piece of his differential equation from the outset. Back to equations (110)–(111), we may infer that the dual least action principle can set a foundation with which to describe other dynamics that are dominated by two independent dynamical causes. In case of the Schrödinger dynamics it is [Least (stationary) action principle for energy quantity] and [Least (stationary) action principle for the wave-flow quantity]. More generally, the functional forms of energy quantity and wave-flow quantity should depend on individual dynamics under study. As an obvious example, the wave-flow quantity in Dirac relativistic theory should not be \( \left\langle \phi \middle| i\hbar \frac{\partial}{\partial t} \frac{\partial \phi}{\partial \phi} \right\rangle \), aside from the four-component wavefunction. This aspect will be discussed elsewhere.

In light of flexibility and structural simplicity of the proposed TDVP, its applications are possible in many areas of quantum dynamics. Among others, applications to nonadiabatic electron wavepacket dynamics in chemical reactions [33], simultaneous electronic and nuclear quantum wave dynamics and relativistic electron dynamics [34, 35] for molecules are under our strong focus. These will be reported in future.

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