Equivalence of time-dependent variational descriptions of quantum systems and Hamilton's mechanics

Kit-Keung Kan*

Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742

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It is shown that any time-dependent description of quantum systems derived from the variational principle is equivalent to Hamilton's description of a classical system. This is done by establishing the fact that the Euler's equations from the variation of the wave function in any parametrization can be transformed to a system of Hamilton's equations. The problem of obtaining collective dynamical variables in quantum many-body systems is discussed in the light of this equivalence.

I. INTRODUCTION

We show in this Communication that any time-dependent description of a quantum system derivable from the variational principle ($\hbar=1$, $\partial_x \equiv \partial/\partial x$)

$$\delta \int_{t_0}^{t_1} \langle \Psi | (i\partial_t - H) | \Psi \rangle dt = 0 \tag{1}$$

for Ψ in an arbitrary manifold in the Hilbert space of normalized wave functions, is equivalent to a classical Hamiltonian system.

For the exact time-dependent Schrödinger description, i.e., for the case that the manifold is the full Hilbert space, such an equivalence is well known.[1] Recently, the interests in large amplitude dynamics of many-body systems have led to active investigations on the variational principle (1) in various types of submanifold. Our knowledge on the equivalence of the variational principle and classical Hamiltonian systems is now widened to include many cases. They are time-dependent Hartree-Fock[2] in which the manifold consists of single Slater determinants, the dynamics derived from manifolds generated by two parameters,[3] and the dynamics derived from manifolds with symplectic structure.[4] Having seen these many cases where the equivalence holds, one may ask whether this equivalence is a general property, valid for any submanifold in the Hilbert space of normalized wave functions. We show in this Communication that it is indeed the case.

In order to show the equivalence of (1) and a classical Hamiltonian system, we utilize parametric representation of the manifold. That is, we consider normalized wave functions Ψ which depend on a set of parameters, such that as these parameters vary, Ψ traces through every element of this manifold. We then show that the variation in an arbitrary manifold can be reduced to the variation in a smaller manifold with a symplectic structure due to the special property of the variational functional that it is linear in the time derivative of the parameters. Then the result on the symplectic manifold[4] can be used to transform the equations of motion to Hamilton's canonical form. However, we present an alternative method for the transformation to canonical form, which has the advantage that it explicitly transforms the variational functional in (1) into a Lagrangian. Thus, the equivalence of (1) and the Hamiltonian system becomes more transparent. The paper concludes with some remarks on the theories of collective dynamics in many-body systems.

II. PROOF OF EQUIVALENCE

A. Euler's equations of motion

In a manifold generated by n real parameters $\vec{\alpha} = (\alpha_1, \ldots, \alpha_n)$, the variational principle (1) can be rewritten as

$$\delta \int_{t_0}^{t_1} \mathfrak{F}\left(\vec{\alpha}, \frac{d\vec{\alpha}}{dt}\right) dt = 0 \ , \tag{2}$$

where the variational functional $\mathfrak{F}$ is

$$\mathfrak{F}\left(\vec{\alpha}\frac{d\vec{\alpha}}{dt}\right) \equiv \langle \Psi(\vec{\alpha}) | (i\partial_t - H) | \Psi(\vec{\alpha}) \rangle$$

$$= i\frac{d\vec{\alpha}}{dt} \cdot \langle \Psi | \partial_{\vec{\alpha}} \Psi \rangle - \langle \Psi | H | \Psi \rangle \ . \tag{3}$$

Only normalized Ψ are considered in this paper.[5-7] The variational principle leads to a set of n Euler's equations of motion for the parameters

$$\partial_{\vec{\alpha}} \mathfrak{F} - \frac{d}{dt} \partial_{d\vec{\alpha}/dt} \mathfrak{F} = 0 \ , \tag{4}$$

which now takes the form

$$\vec{B}(\vec{\alpha}) \frac{d\vec{\alpha}}{dt} = \partial_{\vec{\alpha}} \langle H \rangle \ . \tag{5}$$

Here, $\langle H \rangle \equiv \langle \Psi | H | \Psi \rangle$ and the matrix $\vec{B}$ is antisymmetric and is given by

$$B_{ij}(\vec{\alpha}) = i(\langle \partial_{\alpha_i}\Psi | \partial_{\alpha_j}\Psi\rangle - \langle \partial_{\alpha_j}\Psi | \partial_{\alpha_i}\Psi\rangle) \quad . \tag{6}$$

It follows that all the variational descriptions with a constant Hamiltonian conserve the average energy $\langle H\rangle$: $d\langle H\rangle/dt$ vanishes by (5) and by the antisymmetry of B.

The objective in this Communication is to transform the equations of motion (5) into a system of Hamiltonian equations.

B. Legendre transformation is impossible

We note first that the procedure of applying the Legendre transformation[8] to cast the Euler's equations (4) or (5) into Hamiltonian canonical form fails here. The Legendre transformation is based on the introduction of a set of canonical conjugates $\vec{p}_\alpha \equiv \partial_{\partial\vec{\alpha}/\partial t}\mathfrak{F}(\vec{\alpha}, \partial\vec{\alpha}/\partial t)$ of $\vec{\alpha}$, and then use $\vec{p}_\alpha$ and $\vec{\alpha}$ as new *independent* variables. However, in the present situation the variational functional $\mathfrak{F}$ in (3) is linear in $\partial\vec{\alpha}/\partial t$. As a result the canonical conjugates $\vec{p}_\alpha$ defined in this way are functions of $\vec{\alpha}$ but not a function of $\partial\vec{\alpha}/\partial t$. Therefore, one cannot use $\vec{p}_\alpha$ to eliminate $\partial\vec{\alpha}/\partial t$ and $\vec{p}_\alpha$ and $\vec{\alpha}$ cannot serve as new independent variables. The Legendre transformation is hence impossible. Nevertheless, as we show in the following, the equations of motion (5) can still be transformed by other means into a set of Hamiltonian equations, although the resulting set will consist of fewer equations than $2n$ as would be the case if the Legendre transformation were possible.

C. Reduction to even number of parameters

Before transforming (5) to Hamiltonian canonical form where the canonical variables always appear in pairs, we first show that the number of parameters can always be reduced whenever this number is odd.[9,10]

If n is odd, then $\det(\vec{B})$ vanishes identically[11] because of the antisymmetry of $\vec{B}$. It follows that there exists a linear combination of the n Euler's equations (5) which vanishes identically. That is, one can find n functions $\vec{a}(\vec{\alpha})$, such that

$$\vec{a}(\vec{\alpha}) \cdot \partial_{\vec{\alpha}}\langle H\rangle = 0 \quad . \tag{7}$$

In fact, Eq. (7) can be transformed to a stationarity condition of the energy in terms of a new variable β by the transformation $(\alpha_1, \ldots, \alpha_n) \rightarrow (\beta, \alpha_2, \ldots, \alpha_n)$ which satisfies the condition

$$\frac{\partial\vec{\alpha}}{\partial\beta} = \vec{a}(\vec{\alpha}) \quad . \tag{8}$$

Then, Eq. (7) will reduce to the stationarity condition

$$\partial_\beta\langle H\rangle = 0 \quad . \tag{9}$$

Therefore, when $\det(\vec{B})$ is zero, the variational principle determines the value of this new parameter β at which the energy of the system is stationary.

We are now left with only $n-1$ parameters and $n-1$ Euler's equations of the same form as (5) to deal with. If the determinant of the matrix $\vec{B}$ in this set of new Euler's equation is zero, we can apply the above procedure of reducing the number of parameters again. At the end of a repeated application of this procedure, we shall have a nonsingular $\vec{B}$, and in that case the number of parameters involved is necessarily even.

For the special case $n=1$, the above result that the variational principle leads to a stationarity condition has been pointed out by Kerman and Koonin.[2] In that case the Euler's equation is in itself the stationarity condition (9) on the single parameter involved.

D. Transformation of $2m$ parameters to m pairs of canonical variables

We now show that the set of Euler's equations (5) for $n=2m$ parameters $\vec{\alpha}$ can be transformed to m pairs of Hamiltonian equations.

When the number of parameters is even, the manifold with an antisymmetric $\vec{B}$ is symplectic.[4] One can use the method of Rowe *et al.*,[4] to transform the equations of motion to Hamiltonian canonical form. We here present an alternative method which is a generalization (and a simplification) of that employed in Ref. 3 for the case of two parameters. This method gives an explicit set of differential equations for the transformation, which can be solved by a power series. It also transforms directly the variational functional to the form of a Lagrangian.

We seek here m pairs of new parameters $\vec{q} \equiv (q_1, \ldots, q_m)$ and $\vec{p} \equiv (p_1, \ldots, p_m)$ satisfying the following conditions:

$$i\langle\Psi|\partial_{\vec{q}}\Psi\rangle = \vec{p} \quad , \tag{10a}$$

$$i\langle\Psi|\partial_{\vec{p}}\Psi\rangle = 0 \quad . \tag{10b}$$

If these new parameters can be found, then the matrix $\vec{B}$ will have elements

$$B_{q_ip_j} = i(\partial_{q_i}\langle\Psi|\partial_{p_j}\Psi\rangle - \partial_{p_j}\langle\Psi|\partial_{q_i}\Psi\rangle) = -\delta_{ij} \quad , \tag{11a}$$

$$B_{q_iq_j} = B_{p_ip_j} = 0 \quad , \tag{11b}$$

for $i,j = 1, \ldots, m$, and the Euler's equations (5) reduce immediately to m pairs of Hamiltonian equations

$$\frac{\partial\vec{q}}{\partial t} = \partial_{\vec{p}}\mathcal{H}(\vec{q}, \vec{p}) \quad , \tag{12a}$$

$$\frac{\partial\vec{p}}{\partial t} = -\partial_{\vec{q}}\mathcal{H}(\vec{q}, \vec{p}) \quad , \tag{12b}$$

with the "classical Hamiltonian" $\mathcal{H}(\vec{q},\vec{p}) = \langle H \rangle$.

We did not initially label the variational functional $\mathcal{F}$ in (2) as a Lagrangian, since it is neither derived from the definition that it is equal to the difference of a kinetic energy and a potential energy, nor is it connected to a Hamiltonian by the Legendre transform. However, after the transformation to canonical variables $\vec{p}$ and $\vec{q}$ such a terminology becomes appropriate. For in terms of $\vec{p}$ and $\vec{q}$, we have

$$\mathcal{F} = \vec{p}\cdot\dot{\vec{q}} - \mathcal{H}(\vec{q},\vec{p}) = \mathcal{L} \quad . \tag{13}$$

In terms of the Lagrangian, the equivalence of the variational principle (1) and Hamiltonian dynamics becomes most transparent, since the Euler's equations obtained from (1) by varying $\vec{q}$ and $\vec{p}$ independently are exactly the set of Hamiltonian equations (12).

Equations (10) are satisfied if and only if we can solve the following $2m$ equations

$$\vec{p}\cdot\partial_{\alpha_i}\vec{q} = f_i(\vec{\alpha}),\quad i=1,\ldots,2m \quad , \tag{14}$$

where the functions,

$$f_i(\vec{\alpha}) \equiv i\langle\Psi|\partial_{\alpha_i}\Psi\rangle \quad , \tag{15}$$

are known and are real as guaranteed by the norm conservation of Ψ. To solve this set of equations one can solve the first m equations algebraically for $\vec{p}$ and substitute the results into the rest, obtaining m equations for $\vec{q}$:

$$\begin{vmatrix} \partial_{\alpha_1}q_1 & \cdots & \partial_{\alpha_1}q_m & f_1 \\ \vdots & & & \\ \partial_{\alpha_m}q_1 & \cdots & \partial_{\alpha_m}q_m & f_m \\ \partial_{\alpha_i}q_1 & \cdots & \partial_{\alpha_i}q_m & f_i \end{vmatrix} = 0 \quad , \tag{16}$$

$$i = m+1,\ldots,2m \quad .$$

This set of first-order partial differential equations can be solved as Cauchy's initial value problem.[12] One can construct a power-series solution[12] of this type of problem about an "initial value" of one variable, α_1, say. That is, at $\alpha_1=0$ we choose for $\vec{q}(\vec{\alpha})$ m arbitrary but fixed functions of the variables $\alpha_2,\alpha_3,\ldots,\alpha_{2m}$. From this choice of "initial values" we can calculate all the partial derivatives of $\vec{q}$, which do not involve the differentiation with respect to α_1. With this information, the set of differential equations (16) and its derivatives will allow one to evaluate $\partial_{\alpha_1}\vec{q}$, $\partial_{\alpha_1}\partial_{\alpha_i}\vec{q}$, $i=1,\ldots,2m$ and all higher derivatives involving α_1. We can then generate a power-series solution $\vec{q}(\vec{\alpha})$ of (16) about $\alpha_1=0$. The conjugate momentum $\vec{p}(\vec{\alpha})$ can be obtained from (14) by direct differentiation.

Thus the equations (14) which define the transformation of the $2m$ arbitrary parameters $\vec{\alpha}$ to $(\vec{q},\vec{p})$ can be solved, and in this new set of parameters the equations of motion (5) are in Hamiltonian canonical form. The equivalence of the variational principle (1) and Hamiltonian system is hence established.

For the case of two parameters (α_1,α_2), Eqs. (14) and (16) reduce to

$$p\frac{\partial q}{\partial\alpha_1} = f_1(\alpha_1,\alpha_2) \quad , \tag{17a}$$

$$p\frac{\partial q}{\partial\alpha_2} = f_2(\alpha_1,\alpha_2) \quad , \tag{17b}$$

and

$$f_2\frac{\partial q}{\partial\alpha_1} - f_1\frac{\partial q}{\partial\alpha_2} = 0 \quad . \tag{18}$$

Equation (18) can be solved by elementary methods.[13] With the solution $q(\alpha_1,\alpha_2)$ from (18), $p(\alpha_1,\alpha_2)$ can be calculated by direct differentiation in either (17a) or (17b), completing the transformation to canonical variables. Comparing with the method presented in Ref. 3 for two parameters, one can see that the present method is simpler.

III. DISCUSSION: REMARKS ON COLLECTIVE DYNAMICS

While our result is completely general and applicable in any field of physics where the variational principle (1) is considered, we point out in particular its consequences on the theory of collective dynamics in many-body systems here.

The basic problem in the theory of collective dynamics is to identify the collective variables and to derive the dynamical equations governing these variables. Some progress[14–17] has been made on this problem in the time-dependent Hartree-Fock in recent years. Villars[14] was the first to construct a two-parameter wave function and to show in the adiabatic approximation that the parameters involved are canonical variables through a pair of Hamiltonian equations. Many authors[17] have followed with similar parametric wave functions.

The proof of equivalence presented here shows that in fact one can always introduce collective parameters in the wave function to describe the deformation of the system and then transform the equations of motion into Hamiltonian canonical form. The new parameters $(\vec{q},\vec{p})$ can be properly called the dynamical collective variables as they are now endowed with a dynamical meaning through the Hamiltonian equations. Villars's parametric wave function[14] is then seen to be one out of many possibilities as there is no restriction in the way of introducing the parameters in our derivation. This freedom may allow one to find alternative canonical collective variables should Villars's commutation condition[14] fail.

Adiabatic assumption is crucial in many recent studies of collective phenomena.[14–17] One advantage of the adiabatic assumption is that it leads to a (classical) collective Hamiltonian quadratic in momenta, so that this Hamiltonian can be requantized by standard techniques.[18] However, we should not limit ourselves from considering more general collective phenomena just because of this advantage. In fact, alternative "requantization" methods for general large-amplitude, nonadiabatic situations have been proposed recently in the gauge-invariant periodic quantization (GIPQ) method[3,7] and in the path integral method.[19]

The present result of equivalence has direct consequences on the GIPQ method, since that method is based on the very same variational principle (1). It is shown in Ref. 7 that in terms of the canonical variables the gauge-invariant periodic quantization condition takes the form of the Bohr-Sommerfeld quantization rule. The wave functions in the GIPQ method are then equivalent to the quantized periodic orbits in certain Hamiltonian systems. This result not only adds physical insight to the GIPQ method but also directs the attention of the researchers in that field to the current research[20] on the periodic orbits of Hamiltonian systems.

Recently, the present author has shown[21] that the collective Hamiltonian for the rotation of the many-body system about a fixed axis can be obtained from the variational principle by use of two parameters, the angle of rotation and its associated current, and that the GIPQ on this parametrization leads to the correct quantization of the angular momentum. This is a very encouraging result. Based on the present result for general parametrization, one may hope to eventually derive the Bohr collective Hamiltonian[22] from a 10-parameter variation, 3 Eulerian angles, 2 intrinsic deformations, and their (5) associated currents.

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*Present address: JAYCOR, 205 South Whiting St., Alexandria, Va. 22304.

[1] L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968), p. 498.

[2] A. K. Kerman and S. E. Koonin, Ann. Phys. (N.Y.) 100, 332 (1976).

[3] K.-K. Kan, J. J. Griffin, P. C. Lichtner, and M. Dworzecka, Nucl. Phys. A332, 109 (1979).

[4] D. J. Rowe, A. Ryman, and G. Rosensteel, Phys. Rev. A 22, 2362 (1980).

[5] Variation of the norm of Ψ leads to the important result that the time evolution of the phase of Ψ is uniquely determined (see Refs. 6 and 7). Since this norm variation can be done independently and a general result for the phase is obtained in Ref. 7, only norm-conserved variations are considered here.

[6] P.C. Lichtner, J. J. Griffin, H. Schultheis, R. Schultheis, and A. B. Volkov, Phys. Lett. 88B, 221 (1979); Phys. Rev. C 20, 845 (1979).

[7] K.-K. Kan, Phys. Rev. C. 24, 279 (1981).

[8] R. Courant and D. Hilbert, *Methods of Mathematical Physics*, (Interscience, New York, 1953), Vol. 1, p. 239.

[9] Some authors (see Refs. 4 and 10) have noticed the distinction between the situation with even and odd parameters but avoided discussing the case with odd number of parameters, or sometimes even insisted that the parameters involved are meaningful only when they are complex.

[10] P. G. Reinhard, N. Rowley, and D. M. Brink, Z. Phys. 266, 149 (1974); P. Kramer and M. Saraceno, *Geometry of Time-Dependent Variational Principle in Quantum Mechanics* (Springer, Berlin, 1981).

[11] R. M. Thrall and L. Tornheim, *Vector Space and Matrices* (Wiley, New York, 1957), p. 152.

[12] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1953), Vol. 2, Chap. 2.

[13] I. Sneddon, *Elements of Partial Differential Equations* (McGraw-Hill, New York, 1957), Chap. 2.

[14] F. M. H. Villars, in *Dynamic Structure of Nuclear States*, edited by D. J. Rowe *et al.* (Univ. of Toronto Press, Toronto, 1972), p. 3: F. Villars, Nucl. Phys. A285, 269 (1977); E. Moya de Guerra and F. Villars, *ibid.* A285, 297 (1977).

[15] D. J. Rowe and R. Bassermann, Can. J. Phys. 54, 1941 (1976).

[16] M. Baranger and M. Veneroni, Ann. Phys. (N.Y.) 114, 123 (1978).

[17] D. M. Brink, M. J. Giannoni, and M. Veneroni, Nucl. Phys. A258, 237 (1976); K. Goeke and P. G. Reinhard, Ann. Phys. (N.Y.) 122, 328 (1978); M. J. Giannoni and P. Quentin, Phys. Rev. C 21, 2060 (1980); T. Marumori, A. Hayaski, T. Tomoda, A. Kuriyama, and T. Masakawa, Prog. Theor. Phys. 63, 1576 (1980); E. J. V. de Passos and A. F. R. de Toledo Piza, Phys. Rev. C 21, 425 (1980).

[18] W. Pauli, in *Handbach der Physik* (Springer, Berlin, 1933), Vol. XXIV/1, p. 120.

[19] H. Reinhardt, Nucl. Phys. A331, 353 (1979); S. Levit, J. W. Negele, and Z. Paltiel, Phys. Rev. C 21, 1603 (1980).

[20] P. H. Rabinowitz, Pure Appl. Math. 31, 157 (1978); A. Weinstein, Ann. Math. 108, 507 (1978); I. Ekeland, J. Diff. Equ. 34, 496 (1979).

[21] K.-K. Kan, Phys. Rev. C 24, 789 (1981).

[22] A. Bohr, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. 26, No. 14 (1952).