Lagrangian Densities and Principle of Least Action in Nonrelativistic Quantum Mechanics

Donald H. Kobe
Department of Physics
University of North Texas
Denton, Texas 76203-1427
USA

February 2, 2008

Abstract

The Principle of Least Action is used with a simple Lagrangian density, involving second-order derivatives of the wave function, to obtain the Schrödinger equation. A Hamiltonian density obtained from this simple Lagrangian density shows that Hamilton’s equations also give the Schrödinger equation. This simple Lagrangian density is equivalent to a standard Lagrangian density with first-order derivatives. For a time-independent system the Principle of Least Action reduces to the energy variational principle. For time-dependent systems the Principle of Least Action gives time-dependent approximations. Using a Hartree product trial wave function for a time-dependent many-boson system, we apply the Principle of Least Action to obtain the Gross-Pitaevskii equation that describes a Bose-Einstein condensate.

1 Introduction

The Lagrangian approach using Hamilton’s Principle of Least (or Stationary) Action has been a unifying principle in almost all areas of physics to obtain dynamical equations \([1]-[3]\). The Hamiltonian approach, on the other hand,
depends on a Lagrangian to obtain a canonical momentum and Hamiltonian. In nonrelativistic quantum mechanics the Hamiltonian approach has dominated, however, because the Schrödinger equation uses the Hamiltonian operator obtained by quantizing the canonical momentum of the particles. The wave function in the Schrödinger equation is a complex function in configuration space. From the wave function a Lagrangian density can be constructed and used in Hamilton’s Principle of Least Action to give the Schrödinger equation. This same procedure is used in relativistic quantum field theory, which is primarily based on the Lagrangian approach because the Lagrangian density is a scalar density [4, 5, 6, 3]. Our approach is different from the Feynman path integral formulation of quantum mechanics that uses a classical particle Lagrangian in the path integral to obtain the propagator [7].

In this paper we discuss a simple Lagrangian density for nonrelativistic quantum mechanics that gives the Schrödinger equation when used in the Principle of Least Action. This Lagrangian density has been called “seemingly artificial” [8] because it involves second-order spatial derivatives and is apparently complex, but it is nevertheless widely used [9–13]. From this Lagrangian density we use the canonical procedure for fields to obtain a canonical momentum conjugate to the wave function as a generalized coordinate and then find a Hamiltonian density. Using these, we show that Hamilton’s equations also give the Schrödinger equation. We then show that this simple Lagrangian density is equivalent to a standard Lagrangian density that is real and has only first derivatives [3]. In addition, we show that for time-independent systems the Principle of Least Action reduces to the energy variational principle of nonrelativistic quantum mechanics [12]. For time-dependent systems the Principle of Least Action can be used with time-dependent trial wave functions to obtain approximate equations and solutions. We apply this method to a system of charged bosons with a Hartree product time-dependent trial wave function to obtain the Gross-Pitaevskii equation [14–16], which is a nonlinear Schrödinger equation that describes a Bose-Einstein condensate [17].

In Section 2 we review the Hamiltonian for a nonrelativistic quantum system of many charged particles in an external electromagnetic field. In Section 3 we give a simple Lagrangian density for the system and show that Hamilton’s Principle of Least Action gives the Schrödinger equation. Using this simple Lagrangian density, we apply the canonical formalism in Section 4 to obtain a Hamiltonian density and show that Hamilton’s equations also
give the Schrödinger equation. In Section 5 we give an elementary derivation of the equation of continuity in configuration space for probability based on the invariance of the Lagrangian density under infinitesimal global gauge transformations. We show in Section 6 that our simple Lagrangian density with second-order spatial derivatives is real and equivalent to the standard one with first-order derivatives. For a time-independent system we show in Section 7 that Hamilton’s Principle reduces to the energy variational principle. For a time-dependent system we show in Sec. 8 that a time-dependent trial wave function may be used in Hamilton’s Principle and then apply it to obtain a time-dependent approximate equation for a many-boson system. The conclusion is given in Section 9.

2 Hamiltonian for a many-particle system

For a system of many charged particles in an electromagnetic field the Lagrangian of the classical system can be used to obtain a particle Hamiltonian by using the canonical procedure [18]. The system is quantized by replacing canonical momenta conjugate to the coordinates by operators satisfying canonical commutation relations [19] and the Hamiltonian then becomes an operator. Because of the sum over all particles, the Hamiltonian operator emphasizes the particle aspect of quantum theory. We review the Hamiltonian here to establish the background and notation.

The Hamiltonian operator $\hat{H}$ for a system of $N$-particles with masses $m_i$ and charges $q_i$ in an external electromagnetic field is

$$\hat{H} = \sum_{i=1}^{N} \left\{ \frac{1}{2m_i} [\hat{p}_i - q_i A(\mathbf{r}_i, t)]^2 + q_i A_0(\mathbf{r}_i, t) \right\} + V(\mathbf{r}_1, ..., \mathbf{r}_N),$$  \hspace{1cm} (1)$$

where $V$ is a conservative potential energy. The canonical momentum operator $\hat{p}_i = -i\hbar \nabla_i = -i\hbar \partial / \partial \mathbf{r}_i$ is conjugate to the coordinate $\mathbf{r}_i$ for particle $i = 1, 2, \ldots, N$. Together the coordinates and canonical momenta satisfy the canonical commutation relations. The external classical electromagnetic field is characterized by a vector potential $\mathbf{A}(\mathbf{r}_i, t)$ with components $A_\alpha(\mathbf{r}_i, t)$ for $\alpha = 1, 2, 3$ and a scalar potential $A_0(\mathbf{r}_i, t)$. From these potentials the electric and magnetic fields can be determined in the usual way.

It is convenient for the rest of the paper to use a more compact notation for the Hamiltonian (1). The $\alpha$-component of the displacement $\mathbf{r}_i$ of particle
$i$ has components $x_{i\alpha}$ for $\alpha = 1, 2, 3$. The $\alpha$-component of the mechanical momentum operator $\hat{P}_i$ for particle $i$ is

$$\hat{P}_{i\alpha} = \hat{p}_{i\alpha} - q_i A_{\alpha},$$

(2)

where the $\alpha$-component of the canonical momentum operator is $\hat{p}_{i\alpha} = -i\hbar \partial / \partial x_{i\alpha} = -i\hbar \partial_{i\alpha}$. Using this notation for mechanical momentum, we can rewrite the Hamiltonian operator (1) as

$$\hat{H} = \frac{1}{2m_i} \hat{p}_{i\alpha}^2 + q_i A_0(r_i, t) + V,$$

(3)

where summation over repeated particle numbers $i$ from 1 to $N$ and repeated component indices $\alpha$ from 1 to 3 is understood.

### 3 Lagrangian density and Hamilton’s Principle

The dynamical equations in almost all areas of physics can be obtained from Hamilton’s Principle of Least Action [1, 2]. For a many-particle system the wave function $\Psi$ in nonrelativistic quantum mechanics is a complex function in a $3N$-dimensional configuration space. In order to use Hamilton’s Principle of Least Action to obtain the Schrödinger equation we need a Lagrangian density. Such a Lagrangian density can be constructed from the wave function, its complex conjugate, and their partial derivatives to any order [20]. Because it involves the wave function, the Lagrangian density emphasizes the wave aspect of quantum theory. The wave function of the nonrelativistic quantum system of $N$ particles is a complex, time-dependent function $\Psi = \Psi(t) = \Psi(r, t) = \Psi(r_1, r_2, ..., r_N, t)$, where the $3N$-dimensional vector $r = (r_1, r_2, ..., r_N)$ is a vector in configuration space.

We postulate a simple Lagrangian density $\mathcal{L}$ for this system in terms of the nonrelativistic wave function $\Psi$ as

$$\mathcal{L} = \Psi^*(i\hbar \partial_t - \hat{H})\Psi,$$

(4)

which depends only on $\Psi^*$, $\Psi$ and its partial derivatives $\partial_t \Psi = \partial \Psi / \partial t$, $\partial_{i\alpha} \Psi = \partial \Psi / \partial x_{i\alpha}$, and $\partial_{i\alpha}^2 \Psi = \partial^2 \Psi / \partial x_{i\alpha}^2$. Any Lagrangian density that gives the correct equation of motion is a valid one, so a Lagrangian density that is complex can still be useful [21]. The Lagrangian density need not have only
first-order derivatives as is sometime thought, but can have derivatives of any order [20]. Nesbet [8] has called the Lagrangian density (4) "seemingly artificial," but it is nevertheless widely used [9]-[13]. The Lagrangian density for the Dirac equation is similar in form [4].

To obtain the dynamical equations from a Lagrangian density we use Hamilton’s Principle of Least Action. Hamilton’s Principle [3] states that the action functional

$$S[\Psi^*, \Psi] = \int dt \int d^{3N}r \mathcal{L}(\Psi, \Psi^*, ...) = \text{Stationary},$$

(5)

where the integration is over all time and all configuration space with an element of volume \(d^{3N}r = d^3r_1 \cdots d^3r_N\). The action (5) is stationary when its variation with respect to either \(\Psi^*\) or \(\Psi\) (or both) is zero. For an arbitrary Lagrangian density \(\mathcal{L}(\Psi, \Psi^*, ...)\) variation with respect to \(\Psi^*\) gives the Euler-Lagrange equation [6]. Boundary conditions at infinity on the variations are chosen such that \(\delta \Psi^*\) and \(\delta \Psi\) vanish sufficiently rapid as \(|t| \to \infty\) and \(r_i \to \infty\) for all \(i\).

When the specific Lagrangian density \(\mathcal{L}\) in Eq. (4) is substituted into Eq. (5) and variation is made with respect to \(\Psi^*\), we obtain

$$\delta S[\Psi^*, \Psi] = \int dt \int d^{3N}r \delta \Psi^* \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \Psi = 0. \quad (6)$$

Since the variation \(\delta \Psi^*\) is arbitrary except for vanishing at the boundaries, Eq. (6) immediately gives the Schrödinger equation

$$\hat{H} \Psi = i\hbar \frac{\partial \Psi}{\partial t}, \quad (7)$$

where the wave function \(\Psi(0)\) must be specified. If the variation of the action is made with respect to \(\Psi\), then integration by parts is necessary and the complex conjugate of the Schrödinger equation is obtained.

## 4 Hamiltonian density and Hamilton’s equations

From the Lagrangian density in Eq. (4) we can obtain the Hamiltonian density by the canonical procedure. The Hamiltonian density can be used to obtain Hamilton’s equations. To be consistent with the Principle of Least
Action, Hamilton’s equations must also give the Schrödinger equation (7), and indeed they do. This section uses functional derivatives and is more detailed for pedagogical purposes.

The definition of the Hamiltonian from the Lagrangian for classical particles may be generalized for fields [18]. The many-particle wave function \( \Psi(\mathbf{r}, t) \), where time \( t \) is a parameter and \( \mathbf{r} \) is a vector in the \( 3N \)-dimensional configuration space, can be considered as a generalized coordinate with a conjugate momentum \( \Pi(\mathbf{r}, t) \) in the canonical formalism. The Hamiltonian density \( \mathcal{H} \) is given by a Legendre transformation [18] to obtain a function of \( \Psi(t) \) and \( \Pi(t) \) from the Lagrangian density \( \mathcal{L} \),

\[
\mathcal{H}(\Pi(t), \Psi(t)) = \Pi(\mathbf{r}, t) \dot{\Psi}(\mathbf{r}, t) - \mathcal{L} (\Psi(t), \dot{\Psi}(t)),
\]

where \( \dot{\Psi}(\mathbf{r}, t) \equiv \partial_t \Psi(\mathbf{r}, t) \). The canonical momentum \( \Pi(\mathbf{r}, t) \) conjugate to the generalized coordinate \( \Psi(\mathbf{r}, t) \) is chosen to eliminate the coefficient of \( \delta \dot{\Psi} \) in the variation of Eq. (8), which gives

\[
\Pi(\mathbf{r}, t) \equiv \left( \frac{\partial \mathcal{L}}{\partial \dot{\Psi}(\mathbf{r}, t)} \right) = i\hbar \Psi^*(\mathbf{r}, t).
\]

Substituting \( \Pi(\mathbf{r}, t) = i\hbar \Psi^*(\mathbf{r}, t) \) and \( \mathcal{L} \) in Eq. (11) into Eq. (3), we find that the Hamiltonian density is \( \mathcal{H} = \Psi^* \hat{H} \Psi \), which is the density of the Hamiltonian operator \( \hat{H} \) in Eq. (1). The spatial integral of the Hamiltonian density is the energy \( \mathcal{E}(t) \) of the system

\[
\mathcal{E}(t) = \int d^{3N} r \ \mathcal{H} = \int d^{3N} r \ \Psi^*(\mathbf{r}, t) \hat{H} \Psi(\mathbf{r}, t).
\]

However, when the integral of the Hamiltonian density in Eq. (10) is written in terms of the canonical momentum \( \Pi(\mathbf{r}, t) = i\hbar \Psi^*(\mathbf{r}, t) \) it can be considered as a Hamiltonian functional \( \mathcal{H}[\Psi(t), \Pi(t)] \) for the system

\[
\mathcal{H}[\Psi(t), \Pi(t)] = \int d^{3N} r \ \mathcal{H}(t) = \frac{1}{i\hbar} \int d^{3N} r \ \Pi(\mathbf{r}, t) \hat{H} \Psi(\mathbf{r}, t).
\]

From the Hamiltonian functional and the Euler-Lagrange equation Hamilton’s equations [3, 22] may be written in a familiar form using functional derivatives.

Hamilton’s first equation for fields is [5]

\[
\dot{\Psi}(\mathbf{x}, t) = \frac{\delta \mathcal{H}[\Psi, \Pi]}{\delta \Pi(\mathbf{x}, t)},
\]
where the left-hand side is $\dot{\Psi} = \partial_t \Psi = \partial \Psi / \partial t$. The right-hand side is the functional derivative of the Hamiltonian functional $\mathcal{H}[\Psi, \Pi]$ with respect to the canonical momentum $\Pi(x, t)$, where $x = (x_1, x_2, ..., x_N)$ is also a $3N$-dimensional vector in configuration space. When the Hamiltonian functional in Eq. (11) is substituted into it, Hamilton’s first equation gives

$$
\dot{\Psi}(x, t) = \frac{\delta}{\delta \Pi(x, t)} \int d^{3N}r \frac{1}{i\hbar} \Pi(r, t) \hat{H} \Psi(r, t),
$$

$$
\partial_t \Psi(x, t) = \frac{1}{i\hbar} \int d^{3N}r \frac{\delta \Pi(r, t)}{\delta \Pi(x, t)} \hat{H} \Psi(r, t),
$$

$$
\frac{\partial \Psi(x, t)}{\partial t} = \frac{1}{i\hbar} \hat{H} \Psi(x, t),
$$

which is the Schrödinger equation (7). The functional derivative of $\Pi(r, t)$ [or $\Psi(r, t)$] with respect to $\Pi(x, t)$ [or $\Psi(x, t)$] in Eq. (13) is a $3N$-dimensional delta function [6],

$$
\frac{\delta \Pi(r, t)}{\delta \Pi(x, t)} = \delta^{(3N)}(r - x).
$$

Integrating over this delta function in Eq. (13), we obtain the Schrödinger equation (7). The dimensions of the delta-function on the right-hand side of Eq. (14) are $(\text{length})^{-3N}$, so the functional derivative $\frac{\delta \Pi(r, t)}{\delta \Pi(x, t)}$ also has the same dimensions, contrary to appearances. Thus, it is only apparent that there is a lack of dimensional consistency in Eqs. (12) and (13).

Hamilton’s second equation is [5]

$$
\ddot{\Pi}(x, t) = -\frac{\delta \mathcal{H}[\Psi, \Pi]}{\delta \Psi(x, t)},
$$

where the left-hand side is $\ddot{\Pi}(x, t) = \partial_t \Pi(x, t) = i\hbar \partial \Psi^* (x, t) / \partial t$ from Eq. (9). The right-hand side is the functional derivative of the Hamiltonian functional with respect to the generalized coordinate $\Psi(x, t)$. Using the Hermiticity of the Hamiltonian, taking the functional derivative inside the integral to obtain
a delta function and integrating, we obtain Hamilton’s second equation,

\[
\dot{\Pi}(x, t) = -\frac{\delta}{\delta \Psi(x, t)} \int d^3r \frac{1}{i\hbar} \Pi(r, t) \hat{H} \Psi(r, t),
\]

\[
\partial_t \Pi(x, t) = -\frac{1}{i\hbar} \int d^3r \hat{H} \Pi(r, t) \frac{\delta \Psi(r, t)}{\delta \Psi(x, t)},
\]

\[
i\hbar \frac{\partial \Psi^*(x, t)}{\partial t} = -\hat{H} \Psi^*(x, t), \tag{16}
\]

which is the complex conjugate of the Schrödinger equation (7). Therefore, Eqs. (13) and (16) show that Hamilton’s equations obtained from the canonical formalism using the Hamiltonian density (8) obtained from the Lagrangian density (4) is consistent with Hamilton’s Principle of Least Action in giving the Schrödinger equation.

5 Conservation of probability

Noether’s theorem states that the invariance of a Lagrangian density under a symmetry operation implies a corresponding conservation law \[21, 23\]. In particular the invariance of Lagrangian density (4) under infinitesimal global gauge transformations gives the equation of continuity for probability \[3, 24\]. Even though this relation is well known, the proof of it at an elementary level for nonrelativistic quantum mechanics in configuration space is not readily available. We give a short derivation of it here to use in the next section.

First consider the variation of the Lagrangian density (14) with respect to \(\delta \Psi\). Using “differentiation by parts” \[udv = \,d(\int u v) = -vdu\] and the Schrödinger equation (7), we obtain

\[
\delta \mathcal{L} = i\hbar \partial_t [\Psi^* \delta \Psi] + i\hbar \frac{2m}{2m_i} \partial_{\alpha} \left( \hat{P}_{\alpha} \Psi^* \delta \Psi + \Psi^* \hat{P}_{\alpha} \delta \Psi \right). \tag{17}
\]

At this point the variation \(\delta \Psi\) is arbitrary. When we obtain \(\delta \Psi\) from an infinitesimal global gauge transformation, we find the equation of continuity for probability.

An infinitesimal global gauge transformation on the wave function \(\Psi\) is

\[
\Psi' = \exp \{i\delta \Gamma / \hbar\} \Psi = \Psi + (i\delta \Gamma / \hbar) \Psi + \cdots, \tag{18}
\]

where \(\delta \Gamma = \sum q_i \delta \Lambda\) is an infinitesimal constant. The vector and scalar potentials are of course unchanged by a constant gauge function \(\delta \Lambda\). The new
The Lagrangian density $\mathcal{L}' = \exp\{-i\delta\Gamma/\hbar\} \mathcal{L} \exp\{i\delta\Gamma/\hbar\} = \mathcal{L}$ is obtained using the new wave function $\Psi'$ in place of $\Psi$ in Eq. (4), so $\delta\mathcal{L} = \mathcal{L}' - \mathcal{L} = 0$. The variation in the wave function $\delta\Psi$ under the transformation (18) is $\delta\Psi = \Psi' - \Psi = (i\delta\Gamma/\hbar)\Psi$ [23]. Substituting this $\delta\Psi$ into Eq. (17) and using $\delta\mathcal{L} = 0$, we obtain a generalized equation of continuity

$$\partial_t \Psi^*\Psi + \frac{1}{2m_i} \partial_{i\alpha} \left[ \Psi (\hat{P}_{\alpha} \Psi)^* + \Psi^* (\hat{P}_{\alpha} \Psi) \right] = 0. \tag{19}$$

This equation can be rewritten as the equation of local probability conservation in configuration space

$$\partial_t \rho(r, t) + \partial_{i\alpha} J_{i\alpha}(r, t) = 0. \tag{20}$$

The probability density $\rho(r, t)$ and probability current density $J_{i\alpha}(r, t)$ in the $3N$-dimensional configuration space are defined respectively as

$$\rho(r, t) = \Psi^*(r, t)\Psi(r, t), \quad J_{i\alpha}(r, t) = \text{Re} \Psi^*(r, t)\hat{v}_{i\alpha}\Psi(r, t), \tag{21}$$

where the velocity operator $\hat{v}_i$ is the mechanical momentum $\hat{P}_i$ divided by the mass $m_i$ for particle $i$, i.e., $\hat{v}_i = \hat{P}_i/m_i$.

6 Standard Lagrangian density

The “standard” Lagrangian density $\mathcal{L}_1$ that gives the Schrödinger equation is real and has only first-order derivatives [3, 21],

$$\mathcal{L}_1 = \frac{1}{2} \left[ \Psi^*(i\hbar \partial_t + \mathcal{L}_1 \Psi) + \Psi(i\hbar \partial_t + \mathcal{L}_1 \Psi)^* \right] - \frac{1}{2m_i} (\hat{P}_{\alpha} \Psi)^* (\hat{P}_{\alpha} \Psi) - \Psi^* [V + q_i A_0(r_i, t)] \Psi, \tag{22}$$

where the subscript on $\mathcal{L}_1$ emphasizes that it has only first-order partial derivatives. The Lagrangian density $\mathcal{L}_1$ in Eq. (22) can be rewritten using differentiation by parts as

$$\mathcal{L}_1 = \mathcal{L} - \frac{i\hbar}{2} \left\{ \partial_t (\Psi^* \Psi) + \frac{1}{m_i} \partial_{i\alpha} \left( \Psi^* \hat{P}_{\alpha} \Psi \right) \right\}. \tag{23}$$
Even though the Lagrangian density $\mathcal{L}$ in Eq. (4) is apparently complex, its imaginary part is zero, which can be shown by taking the imaginary part of Eq. (23),

$$\text{Im} \mathcal{L} = \frac{\hbar}{2} \left\{ \partial_t (\Psi^* \Psi) + \frac{1}{m_i} \partial_{\alpha i} \text{Re} (\Psi^* P_{\alpha i} \Psi) \right\} = 0,$$

(24)

from the equation of continuity (19). The real part of $\mathcal{L}$ in Eq. (23) is

$$\text{Re} \mathcal{L} = \mathcal{L} = \mathcal{L}_1 - \frac{\hbar}{2m_i} \partial_{\alpha i} \text{Im} (\Psi^* \hat{P}_{\alpha i} \Psi),$$

(25)

so the Lagrangian densities $\mathcal{L}$ and $\mathcal{L}_1$ are not equal. Nevertheless, they are equivalent to each other in the sense that they have the same action [21]. Their difference is a partial derivative with respect to the spatial coordinates which vanishes because of boundary conditions when integrated to obtain the action (5). The same dynamical equation, viz., the Schrödinger equation, is therefore obtained from both Lagrangian densities.

Sil [26] was the first to use the real part of $\mathcal{L}$ as a Lagrangian density,

$$\mathcal{L}_{\text{Sil}} = \text{Re} \Psi^* \left( i \hbar \partial_t - \hat{H} \right) \Psi = \text{Re} \mathcal{L},$$

(26)

which was later used by Mittleman [27]. It was subsequently used by McCarroll, et al. [28], who pointed out that $\text{Re} \mathcal{L} = \mathcal{L}$.

### 7 Energy Variational Principle

If the quantum mechanical system is time independent then Hamilton’s Principle reduces to the energy variational principle of time-independent quantum mechanics [12]. The time-independent Schrödinger equation can be obtained by separation of the time variable in the time-dependent Schrödinger equation. However, the time-independent Schrödinger equation can also be obtained from Hamilton’s principle by using it with a trial wave function.

The Principle of Least Action can be used with a trial wave function of the form

$$\Psi(r_1, r_2, \ldots r_N, t) = \Psi(r_1, r_2, \ldots r_N) \exp \left( -iEt/\hbar - \epsilon |t| \right),$$

(27)

where $\Psi$ on the right-hand side is time independent, $E$ is the energy and $\epsilon > 0$ is a small parameter that can be taken to be zero at the end of the
calculation. Using this wave function in Eq. (5) for the action and doing the time integration, we obtain

$$S[\Psi^*, \Psi] = \frac{1}{\epsilon} \int d^3 N \Psi^* \left( E - \hat{H} \right) \Psi = \text{Stationary.} \quad (28)$$

If this equation is multiplied by $-\epsilon < 0$ and the constant $E$ is added, we obtain the energy variational principle for a stationary state

$$\int d^3 N \Psi^* \hat{H} \Psi - E (\int d^3 N \Psi^* \Psi - 1) = \text{Stationary}, \quad (29)$$

which is independent of $\epsilon$. The energy $E$ is a Lagrangian multiplier that ensures the normalization of the wave function.

If the variation of Eq. (29) is made with respect to the function $\Psi^*$, we obtain the time-independent Schrödinger equation

$$\hat{H} \Psi = E \Psi. \quad (30)$$

The variation with respect to $\Psi$ gives the complex conjugate of the time-independent Schrödinger equation (30) after integration by parts.

Hamilton’s Principle of Least Action is however more important in obtaining approximate solutions for the energy and wave function. If the wave function $\Psi$ in Eq. (29) is replaced by a time-independent normalized trial wave function $\Phi$ with parameters or unknown functions and an energy $\langle \Phi | \hat{H} \Phi \rangle = E'$. Then Eq. (29) can be varied with respect to these parameters or functions to obtain the lowest energy $E'$ with a wave function of the form $\Phi$.

From the standard Rayleigh-Ritz method it is easy to show that the energy $\langle \Phi | \hat{H} \Phi \rangle = E'$ is an upper bound to the true ground state energy $E_0$, i.e., $E' > E_0$. \[19\]

8 Time-dependent approximation for a many-particle system

Approximate solutions or equations for the time-dependent Schrödinger equation (7) can be obtained from the Principle of Least Action (5) by using the Lagrangian density (4) and replacing the exact wave function $\Psi(t)$ in by a
time-dependent trial wave function $\Phi(t)$,

$$S[\Phi^*, \Phi] = \int dt \int d^3 r \Phi^*(t) \left( i \hbar \partial_t - \hat{H} \right) \Phi(t) = \text{Stationary}, \quad (31)$$

and varying with respect to parameters or functions in $\Phi(t)$. Equation (31) can be used to obtain a time-dependent approximation for any quantum system regardless of the number of particles.

For $N$-identical particles with $q_i = q$ and $m_i = m$, the potential energy $V$ in the Hamiltonian (1) is taken to be the sum of one- and two-body potentials

$$V(r_1, r_2, ..., r_N) = \sum_{i=1}^{N} V^{(1)}(r_i) + \frac{1}{2} \sum_{i \neq j=1}^{N} V^{(2)}(r_i, r_j), \quad (32)$$

respectively, where the two-body potential is symmetric $V^{(2)}(r_i, r_j) = V^{(2)}(r_j, r_i)$. This form of the Principle of Least Action is applicable to any system of many identical particles, either bosons or fermions.

We illustrate Hamilton’s Principle with an approximate wave function for a system of many bosons to obtain the Gross-Pitaevskii equation [14]-[16], which is a nonlinear Schrödinger equation commonly used to treat Bose-Einstein condensates [17]. We choose a time-dependent trial wave function $\Phi(t)$ for a system of $N$-identical bosons as a Hartree product of identical, normalized single-particle functions $\varphi(r, t)$,

$$\Phi(r_1, r_2, ..., r_N, t) = \varphi(r_1, t) \varphi(r_2, t) \cdots \varphi(r_N, t), \quad (33)$$

which satisfies Bose-Einstein statistics because it is symmetric under interchange of particles. Substituting Eq. (33) into the variational principle (31) and integrating over the coordinates, we obtain the action functional in terms of single boson wave functions $\varphi$

$$S [\varphi^*, \varphi] = N \int dt \int d^3 r \varphi^*(r, t) \left\{ i \hbar \partial_t \varphi(r, t) - \frac{1}{2m} [-i \hbar \nabla - q A]^2 \varphi(r, t) - q A_0 \varphi(r, t) - V^{(1)}(r) \varphi(r, t) - \frac{1}{2} (N - 1) \int d^3 r' V^{(2)}(r, r') \varphi^*(r', t) \varphi(r', t) \varphi(r, t) \right\}$$

$$= \text{Stationary}, \quad (34)$$
where the integration is over all time and space.

Variation of this expression with respect to $\varphi^*$ gives a time-dependent Hartree approximation known as the Gross-Pitaevskii equation [14]-[16],

$$i\hbar \frac{\partial}{\partial t} \varphi(r, t) = \frac{1}{2m} \left[ -i\hbar \nabla - q A(r, t) \right]^2 \varphi(r, t) + [q A_0(r, t) + V^{(1)}(r)] \varphi(r, t)$$

$$+ (N - 1) \int d^3 r' V^{(2)}(r, r') \varphi^*(r', t) \varphi(r', t) \varphi(r, t),$$

(35)

for a charged many-boson system in an electromagnetic field [29]. This equation is a nonlinear Schrödinger equation for the single boson wave function $\varphi$, where the nonlinear term is the average potential on one particle due to all the other particles in the system. The variation may also be made with respect to $\varphi(r, t)$ to obtain the complex conjugate of Eq. (35).

9 Conclusion

Hamilton’s Principle of Least Action is a fundamental principle of physics that is used to obtain dynamical equations for both nonrelativistic and relativistic particles and fields [1, 2]. This principle is applied to nonrelativistic quantum mechanics by considering the wave function in configuration space as a generalized coordinate and constructing a Lagrangian density such that Hamilton’s Principle gives the Schrödinger equation. This approach gives a unified treatment for both nonrelativistic quantum theory and relativistic quantum field theory [4], as well as showing their unity with other branches of physics. The Lagrangian approach is in a sense more fundamental than the Hamiltonian approach that has dominated the treatment of nonrelativistic quantum mechanics because the Hamiltonian must be derived from a Lagrangian. In relativistic theory the Lagrangian density is also a scalar density, whereas the Hamiltonian density is not. The two approaches are, however, complementary in the sense that the Lagrangian density using the wave function emphasizes the wave aspect of nature, whereas the Hamiltonian operator with a sum over particles emphasizes its particle aspect.

We use a simple Lagrangian density for the Schrödinger equation that is apparently complex and has second-order spatial derivatives. This Lagrangian density is actually real because of the equation of continuity for probability. It is equivalent to the standard Lagrangian density that is real
and has only first-order derivatives [21]. Two Lagrangian densities are equivalent if the difference between the two is a sum of spatial or temporal partial derivatives so they give the same action.

For time-independent quantum systems, the Principle of Least Action reduces to the energy variational principle of nonrelativistic quantum mechanics. By minimizing the energy calculated from a trial wave function, it gives an approximate wave function and an energy that is an upper bound to the exact ground state energy.

For time-dependent quantum systems, the Principle of Least Action with a time-dependent trial wave function gives an approximate equation for the trial wave function. We apply this approach to a many boson system by using a Hartree product wave function to obtain the time-dependent Gross-Pitaevskii equation [14]–[16], which is a nonlinear Schrödinger equation that describes a Bose-Einstein condensate [17]. For fermion systems a Slater determinant with time-dependent single-particle trial wave functions may be used to obtain the time-dependent Hartree-Fock equations [8].

The Lagrangian approach to nonrelativistic quantum mechanics described here would be suitable to supplement a course in quantum mechanics or field theory. For quantum mechanics it would show how to obtain time-dependent approximations. For field theory it would be a simple familiar example. For both its use would show the unity that Hamilton’s Principle of Least Action provides for physics [1]–[3].

10 Acknowledgements

This paper is dedicated to the memory of my father Kenneth A. Kobe (1905-1958), Professor of Chemical Engineering at the University of Texas, Austin, who encouraged me to pursue my interest in physics.

I would like to thank Professor Wolfgang P. Schleich and Dr. Reinhold Waizer for discussions and Professor Marlan O. Scully for his encouragement. This work was partially supported by a grant from ONR N00014-03-1-0639/TAMU TEES 53494.
References

[1] Lanczos C 1970 The Variational Principles of Mechanics, 4th edn (Toronto: University of Toronto Press) Reprinted: 1986 (New York: Dover Publications)

[2] Yourgrau W and Mandelstam S 1968 Variational Principles in Dynamics and Quantum Theory, (Philadelphia: Saunders) Reprinted: 1979 (New York: Dover Publications)

[3] Moiseiwitsch B L 1966 Variational Principles (New York: Interscience Publishers) pp 77-78, 81-83, 115-119

[4] Lurie D 1968 Particles and Fields (Interscience Publishers: New York) Chap 2, p 58

[5] Weinberg S 1995 The Quantum Theory of Fields. Vol.1, Foundations (Cambridge: Cambridge University Press) pp 298-305

[6] Ryder L H 1985 Quantum Field Theory (Cambridge: Cambridge University Press) pp 84-89, 176-178

[7] Feynman R P and Hibbs A R 1965 Quantum Mechanics and Path Integrals (New York: McGraw-Hill Book Company)

[8] Nesbet R K 2003 Variational Principles and Methods in Theoretical Physics and Chemistry (Cambridge: Cambridge University Press) Chap 6

[9] Moccia R 1973 Time-dependent variational principle Int. J. Quantum Chem. 7 779-783

[10] Gray C G, Karl C and Novikov V A 2004 Progress in classical and quantum variational principles Rept. Prog. Phys. 67 159-208

[11] Deumens E, Diz A, Longo R and Öhrn Y 1994 Time-dependent theoretical treatments of the dynamics of electrons and nuclei in molecular systems Rev. Mod. Phys. 66 917-983 See especially Section II.D.

[12] Sigmund P and Basbas G 1985 A time-dependent analog of the Ritz variational principle in nonrelativistic quantum mechanics Phys. Scripta 32 482-485
[13] Kramer P and Saraceno M 1981 *Geometry of the Time-Dependent Variational Principle in Quantum Mechanics* (Berlin: Springer-Verlag) Chap. 2

[14] Gross E P 1958 Classical theory of boson wave fields *Ann. Phys. (N. Y.)* 4 57-74; Gross E P 1960 Quantum theory of interacting bosons *Ann. Phys. (N. Y.)* 9 292-324

[15] Pitaevskii L P 1961 Vortex lines in an imperfect bose gas *Zh. Eksperim. Teor. Fiz.* 40 646-651; Translation: 1961 *Sov. Phys. JETP* 13 451-454

[16] Kobe D H 1972 Gross-Pitaevski equation for a strongly interacting superfluid boson system *Phys. Rev. A* 5 854-861

[17] Cornell E A and Wieman C E 2002 Nobel Lecture: Bose-Einstein condensation in a dilute gas, the first 70 years and some recent experiments *Rev. Mod. Phys.* 74, 875-893

[18] Goldstein H, Poole C and Safko J 2002 *Classical Mechanics, 3rd ed.* (San Francisco: Addison Wesley) pp 334-343, 573

[19] Merzbacher E 1998 *Quantum Mechanics, 3rd ed.* (New York: Wiley) pp 25-38, 135-142

[20] Brown G J N, O’Rourke S F C and Crothers D S F 1994 Variational principles and second-order Lagrangian densities *Physica Scripta* 49 129-134

[21] Brown H R and Holland P 2004 Simple applications of Noether’s first theorem in quantum mechanics and electromagnetism *Am. J. Phys.* 72 34-39

[22] Doughty N A 1990 *Lagrangian Interaction* (New York: Addison-Wesley) pp 178-179, 214-216, 234

[23] Hill E L 1951 Hamilton’s Principle and the Conservation Theorems of Mathematical Physics *Rev. Mod. Phys.* 23 253-260

[24] Sakurai J J 1977 *Advanced Quantum Mechanics* (Reading, MA: Addison-Wesley) p 10 He deals with a relativistic complex scalar field.
[25] Schweber S S 1961 *An Introduction to Relativistic Quantum Field Theory* (New York: Harper and Row) pp 207-211

[26] Sil N C 1960 Electron capture by protons passing through hydrogen *Proc. Phys. Soc.* 75 194-200

[27] Mittleman M H 1963 Proton-hydrogen scattering systems *Phys. Rev.* 122 499-506

[28] McCarroll R, Piacentini R D and Salin A 1970 Differential cross sections in proton-hydrogen collisions *J. Phys. B: Atom. Molec. Phys.* 3 137-148

[29] Reinisch G 2004 Nonlinear quantization of a degenerate Bose gas in an external Coulomb trap *Phys. Rev. A* 70 033613-1-11