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From Generalized Hamilton Principle to Generalized Schrodinger Equation

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Abstract

The Hamilton principle is a variation principle describing the isolated and conservative systems, its Lagrange function is the difference between kinetic energy and potential energy. By Feynman path integration, we can obtain the standard Schrodinger equation. In this paper, we have given the generalized Hamilton principle, which can describe the heat exchange system, and the nonconservative force system. On this basis, we have further given their generalized Lagrange functions and Hamilton functions. With the Feynman path integration, we have given the generalized Schrodinger equation of nonconservative force system and the heat exchange system.

Keywords

Generalized Hamilton Principle, Nonconservative Systems, Thermodynamic System, Generalized Schrodinger Equation

1. Introduction

In quantum mechanics, each classical physical quantity corresponds to an operator, and the operator has a real eigenvalue, which is guaranteed by the Hermitian operator. The Hermitian operator has always been generally considered to represent observable measurements. In fact, in quantum mechanics, it is only necessary to guarantee the observability of the mechanical quantity, but not to guarantee that its operator must be Hermitian, that is, observable measurement may also be non-Hermitian. In 1947, in order to solve the divergence problem in the field theory, Pauli used the indeterminate metric to put forward the theory of the non-Hermitian operator and its self-consistent inner product, which was derived from a field quantization method proposed by Dirac [1] [2]. In order to maintain the unitary nature of the S matrix, Lee and Wick applied the non-

Hermitian view to quantum electrodynamics [3]. Later, in different fields, numerous studies have proved that under certain conditions, the non-Hermitian Hamiltonian quantum has a real number energy spectrum [4] [5] [6] [7]. In 1998, the author Bender proposed the space-time inverse symmetry (PT symmetry) quantum mechanics, which made the non-Hermitian quantum mechanics have a great leap forward [8] [9]. The non-Hermitian PT symmetric Hamilton do not violate the physical principles of quantum mechanics and have real eigenvalues. Over the past decade PT symmetric quantum theory has been developed into a variety of studies, including field theory and high-energy particle physics. Recently, preliminary studies on PT symmetric systems under optical structures have been carried out.

The quantum theory of non-Hermitian is described dissipative systems and open systems, their unique properties have attracted fast growing interest in the last two decades [10] [11] [12] [13], especially those empowered by parity-time symmetry. While the non-Hermitian quantum theories is still under intense investigation, its application in different fields has led to a plethora of findings, ranging from nonlinear dynamics [14], atomic physics [15], photonics [16], acoustics [17], microwave [18], electronics [19], to quantum information science [20].

The Hamilton principle is a variation principle describing the isolated and conservative systems, its Lagrange function is the difference between kinetic energy and potential energy. By Feynman path integration, we can obtain the standard Schrodinger equation. In this paper, we have given the generalized Hamilton principle, which can describe the heat exchange system, and the non-conservative force system. On this basis, we have further given their generalized Lagrange functions and Hamilton functions. With the Feynman path integration, we have given the generalized Schrodinger equation of nonconservative force system and the heat exchange system.

2. The Hamilton Principle for the Conservative System

In a mechanical system, the constraints that limit its position and speed can be written as equations

$$f\left(\boldsymbol{r}_i,\dot{\boldsymbol{r}}_i,t\right)=0,\quad \left(i=1,2,\cdots,h\right) \tag{1}$$

the number of constraints equations are h. For the mechanical system of N free particles, their degree of freedom is $3N$, when they are restricted by h constraints of Equation (1), we can select $3N-h$ generalized coordinates $q_1,q_2,\cdots,q_{3N-h}$, the position vector $\boldsymbol{r}_i$ can be written as

$$\boldsymbol{r}_i=\boldsymbol{r}_i\left(q_1,q_2,\cdots,q_{3N-h},t\right),\quad \left(i=1,2,\cdots,N\right) \tag{2}$$

the generalized coordinates q_i constitute the configuration space of $3N-h$ dimension

$$\boldsymbol{q}=\left[q_1,q_2,\cdots,q_{3N-h}\right], \tag{3}$$

the virtual displacement are

$$\delta \boldsymbol{q} = \left[\delta q_1, \delta q_2, \cdots, \delta q_{3N-h}\right], \tag{4}$$

the generalized velocity is

$$\dot{\boldsymbol{q}} = \frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \left[\dot{q}_1, \dot{q}_1, \cdots, \dot{q}_{3N-h}\right], \tag{5}$$

where $\dot{q}_i = \frac{\mathrm{d}q_i}{\mathrm{d}t}$.

With Equation (2), we have

$$\delta \boldsymbol{r}_i = \sum_j \frac{\partial \boldsymbol{r}_i}{\partial q_j} \delta q_j, \tag{6}$$

with Equation (6), we can calculate the virtual work of active force $\boldsymbol{F}_i$, it is

$$\delta \omega = \sum_i^N \boldsymbol{F}_i \cdot \delta r_i = \sum_i \boldsymbol{F}_i \cdot \sum_j \frac{\partial \boldsymbol{r}_i}{\partial q_j} \delta q_j = \sum_j \left(\sum_i \boldsymbol{F}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} \right) \delta q_j = \sum_j Q_j \delta q_j, \tag{7}$$

the generalized force Q_j is

$$Q_j = \sum_i \boldsymbol{F}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j}, \tag{8}$$

if the generalized force Q_j is conservative force, the Equation (7) becomes

$$\delta \omega = \sum_j Q_j \delta q_j = -\delta U, \tag{9}$$

where U is the potential energy.

In rectangular coordinates, there is

$$\boldsymbol{F} = -\nabla U, \tag{10}$$

and the component is

$$F_i = -\frac{\partial U}{\partial x}. \tag{11}$$

In the following, we should study the system motion from time t_1 to t_2, the T is the system kinetic energy, there is

$$\int_{t_1}^{t_2} T\mathrm{d}t = \int_{t_1}^{t_2} T\left(q_i, \dot{q}_i, t\right)\mathrm{d}t, \tag{12}$$

where $T = \sum_i \frac{1}{2} m_i \boldsymbol{v}_i^2$.

The variation of Equation (12) is

$$\delta \int_{t_1}^{t_2} T\mathrm{d}t = \int_{t_1}^{t_2} \delta T\mathrm{d}t = \int_{t_1}^{t_2} \sum_i m_i \boldsymbol{v}_i \cdot \delta \boldsymbol{v}_i \mathrm{d}t, \tag{13}$$

with $\boldsymbol{v}_i = \frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t}$, we have

$$\delta \boldsymbol{v}_i = \frac{\mathrm{d}\left(\delta \boldsymbol{r}_i\right)}{\mathrm{d}t} \tag{14}$$

the Equation (13) becomes

$$\delta \int_{t_1}^{t_2} T\mathrm{d}t = \int_{t_1}^{t_2} \sum_i m_i \boldsymbol{v}_i \cdot \frac{\mathrm{d}\left(\delta \boldsymbol{r}_i\right)}{\mathrm{d}t} \mathrm{d}t = \sum_i m_i \boldsymbol{v}_i \cdot \delta \boldsymbol{r}_i \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \sum_i m_i \dot{\boldsymbol{v}}_i \cdot \delta \boldsymbol{r}_i \mathrm{d}t \tag{15}$$

i.e.,

$$\delta\int_{t_1}^{t_2} T\mathrm{d}t+\int_{t_1}^{t_2}\sum_i m_i\dot{\boldsymbol{v}}_i\cdot\delta\boldsymbol{r}_i\mathrm{d}t=\sum_i m_i\dot{\boldsymbol{v}}_i\cdot\delta r_i\Big|_{t_1}^{t_2} \tag{16}$$

with $\boldsymbol{F}_i=m_i\dot{\boldsymbol{v}}_i$ and $\delta\omega=\sum_i\boldsymbol{F}_i\cdot\delta r_i$, we have

$$\delta\int_{t_1}^{t_2} T\mathrm{d}t+\int_{t_1}^{t_2}\sum_i \boldsymbol{F}_i\cdot\delta\boldsymbol{r}_i\mathrm{d}t=\sum_i m_i\dot{\boldsymbol{v}}_i\cdot\delta r_i\Big|_{t_1}^{t_2} \tag{17}$$

and

$$\delta\int_{t_1}^{t_2} T\mathrm{d}t+\int_{t_1}^{t_2}\delta\omega\mathrm{d}t=\sum_i m_i\dot{\boldsymbol{v}}_i\cdot\delta r_i\Big|_{t_1}^{t_2}, \tag{18}$$

if the variation of two endpoints are zero, there are

$$\delta q_j\Big|_{t_1}=\delta q_j\Big|_{t_2}=0 \tag{19}$$

and

$$\delta\boldsymbol{r}_i\Big|_{t_1}=\delta\boldsymbol{r}_i\Big|_{t_2}=0 \tag{20}$$

the Equation (18) becomes

$$\delta\int_{t_1}^{t_2} T\mathrm{d}t+\int_{t_1}^{t_2}\delta\omega\mathrm{d}t=0, \tag{21}$$

as the kinetic energy T is determined by the speed of each moment, there is

$$\delta\int_{t_1}^{t_2} T\mathrm{d}t=\int_{t_1}^{t_2}\delta T\mathrm{d}t. \tag{22}$$

When the active force F is conservative force, the work it does can be expressed as potential energy U, it is

$$\int_{t_1}^{t_2}\boldsymbol{F}\cdot\delta\boldsymbol{r}\mathrm{d}t=\int_{t_1}^{t_2}\delta\omega\mathrm{d}t=-\int_{t_1}^{t_2}\delta U\mathrm{d}t=-\delta\int_{t_1}^{t_2}U\mathrm{d}t, \tag{23}$$

the Equation (21) becomes

$$\delta\int_{t_1}^{t_2}(T-U)\mathrm{d}t=0, \tag{24}$$

i.e.,

$$\delta\int_{t_1}^{t_2}L\mathrm{d}t=0, \tag{25}$$

or

$$\delta S=0. \tag{26}$$

where the Lagrange function $L=T-V$, and the action $S=\int_{t_1}^{t_2}L\mathrm{d}t$. The Equation (25) or (26) is the Hamilton principle for the conservative system.

3. The Generalized Hamilton Principle for the Nonconservative System

When the active forces include both conservative force F_1 and nonconservative force F_2, we have

$$\delta\omega=\boldsymbol{F}_1\cdot\delta\boldsymbol{r}+\boldsymbol{F}_2\cdot\delta\boldsymbol{r}=\delta\omega_1+\delta\omega_2, \tag{27}$$

and

$$\int_{t_1}^{t_2} \boldsymbol{F}_1 \cdot \delta \boldsymbol{r} \mathrm{d}t = \int_{t_1}^{t_2} \delta\omega_1 \mathrm{d}t = -\int_{t_1}^{t_2} \delta U \mathrm{d}t = -\delta \int_{t_1}^{t_2} U \mathrm{d}t, \tag{28}$$

substituting Equations (27) and (28) into (21), there are

$$\delta \int_{t_1}^{t_2} (T - U) \mathrm{d}t + \int_{t_1}^{t_2} \delta\omega_2 \mathrm{d}t = 0, \tag{29}$$

and

$$\int_{t_1}^{t_2} \delta (T - U) \mathrm{d}t + \int_{t_1}^{t_2} \delta\omega_2 \mathrm{d}t = 0, \tag{30}$$

or

$$\int_{t_1}^{t_2} \delta (T - U + \omega_2) \mathrm{d}t = 0, \tag{31}$$

we define generalized Lagrange function $\bar{L}$, it is

$$\bar{L} = T - U + \omega_2 = L + \omega_2, \tag{32}$$

the Equation (31) becomes

$$\int_{t_1}^{t_2} \delta \bar{L} \mathrm{d}t = \int_{t_1}^{t_2} \delta (L + \omega_2) \mathrm{d}t = \int_{t_1}^{t_2} (\delta L + \delta\omega_2) \mathrm{d}t = 0. \tag{33}$$

The Equation (33) is called the generalized Hamilton principle for the nonconservative force system, it is different from the Hamilton principle (25) for the conservative force system, the Equation (33) contains the work of nonconservative force, and the variation is inside the integral sign.

From Equation (7), we can give the work of nonconservative forces $F_{2i} (i = 1, 2, \cdots, N)$, it is

$$\delta\omega_2 = \sum_{i=1}^{N} \boldsymbol{F}_{2i} \cdot \delta \boldsymbol{r}_i = \sum_j \left(\sum_i \boldsymbol{F}_{2i} \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} \right) \delta q_j = \sum_i \left(\sum_{j=1}^{N} \boldsymbol{F}_{2j} \cdot \frac{\partial \boldsymbol{r}_j}{\partial q_i} \right) \delta q_i, \tag{34}$$

when there is a single nonconservative force F_2, there is

$$\delta\omega_2 = \sum_i \boldsymbol{F}_2 \cdot \frac{\partial \boldsymbol{r}}{\partial q_i} \delta q_i = \sum_i F_{2i} \delta q_i. \tag{35}$$

So, when there are both conservative force F_1 and nonconservative force F_2 for the system, the generalized Lagrange function is

$$\bar{L} = T - U + \omega_2 = L + \int \boldsymbol{F}_2 \cdot \mathrm{d}\boldsymbol{r}, \tag{36}$$

the generalized action is

$$\bar{S} = \int_{t_1}^{t_2} \bar{L} \mathrm{d}t. \tag{37}$$

and the generalized Hamilton principle is

$$\int_{t_1}^{t_2} \delta \bar{L} \mathrm{d}t = \int_{t_1}^{t_2} (\delta L + \delta\omega_2) \mathrm{d}t = 0. \tag{38}$$

when there is only nonconservative force F_2, and there is not conservative force F_1 for the system, the generalized Hamilton principle is

$$\int_{t_1}^{t_2} \delta \bar{L} \mathrm{d}t = \int_{t_1}^{t_2} (\delta T + \delta\omega_2) \mathrm{d}t = 0, \tag{39}$$

and the generalized Lagrange function is

$$\bar{L} = T + \omega_2 = T + \int \boldsymbol{F}_2 \cdot \mathrm{d}\boldsymbol{r}. \tag{40}$$

4. The Generalized Hamilton Principle for the Heat Exchange System

In the mechanical, the change rate of energy is

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \boldsymbol{F} \cdot \boldsymbol{v}. \tag{41}$$

For a microcosmic particle, when it exchanges heat Q with the outside world, there is

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\mathrm{d}Q}{\mathrm{d}t}, \tag{42}$$

and the radiant force should be produced, it is

$$\boldsymbol{F} \cdot \boldsymbol{v} = \frac{\mathrm{d}Q}{\mathrm{d}t}, \tag{43}$$

when the microcosmic particle absorb heat, $\frac{\mathrm{d}Q}{\mathrm{d}t} > 0$, the radiant force is $\boldsymbol{F} = -k\boldsymbol{v}$. When the microcosmic particle deliver heat, $\frac{\mathrm{d}Q}{\mathrm{d}t} < 0$, the radiant force is $\boldsymbol{F} = k\boldsymbol{v}$. The Equation (43) should be changed to the following formula

$$\boldsymbol{F} \cdot \boldsymbol{v} = -\frac{\mathrm{d}Q}{\mathrm{d}t}, \tag{44}$$

i.e.,

$$\boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r} = \boldsymbol{F} \cdot \boldsymbol{v}\mathrm{d}t = -\mathrm{d}Q, \tag{45}$$

then

$$\int \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r} = -\int \mathrm{d}Q = -Q, \tag{46}$$

the radiant force is a nonconservative force, When a microcosmic particle exchanges heat with the outside world, its generalized Lagrange function is

$$\bar{L} = T - U + \int \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r} = L - Q, \tag{47}$$

the generalized Hamiltonian function for the heat exchange system is

$$\bar{H} = p\dot{q} - \bar{L} = T + U + Q, \tag{48}$$

and the generalized Hamilton principle for the heat exchange system is

$$\int_{t_1}^{t_2} \delta\bar{L}\mathrm{d}t = \int_{t_1}^{t_2} \left(\delta L - \delta Q\right)\mathrm{d}t = 0. \tag{49}$$

5. The Generalized Lagrange Equation and Generalized Hamilton Function for the Nonconservative System

1) The generalized Lagrange equation for the nonconservative system

For the nonconservative system, the generalized Lagrange function is

$$\bar{L} = T - U + \omega_2 = L + \omega_2 = L + \int \boldsymbol{F}_2 \cdot \mathrm{d}\boldsymbol{r}, \tag{50}$$

i.e.,

$$\bar{L} = L(q_i, \dot{q}_i, t) + \omega_2(\boldsymbol{r}(q_i), t), \tag{51}$$

the variation of $\bar{L}$ is

$$\begin{aligned}\delta\bar{L} &= \delta L(q_i, \dot{q}_i, t) + \delta\omega_2(\boldsymbol{r}(q_i), t)\\ &= \frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i + \boldsymbol{F}_2 \cdot \delta\boldsymbol{r}\\ &= \frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i + \boldsymbol{F}_2 \cdot \frac{\partial \boldsymbol{r}}{\partial q_i}\delta q_i\\ &= \frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i + F_{2i} \cdot \delta q_i,\end{aligned} \tag{52}$$

where $\delta\omega_2 = \boldsymbol{F}_2 \cdot \delta\boldsymbol{r}$, $\delta\boldsymbol{r} = \frac{\partial \boldsymbol{r}}{\partial q_i}\delta q_i$ and $\boldsymbol{F}_2 \cdot \frac{\partial \boldsymbol{r}}{\partial q_i} = F_{2i}$.

Substituting Equation (52) into the generalized Hamilton principle (38), there is

$$\int_{t_1}^{t_2} \delta\bar{L}\mathrm{d}t = \int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i + F_{2i} \cdot \delta q_i\right)\mathrm{d}t = 0. \tag{53}$$

Obviously, there is

$$\int_{t_1}^{t_2} \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i\mathrm{d}t = -\int_{t_1}^{t_2} \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i}\delta q_i\mathrm{d}t \tag{54}$$

substituting Equation (54) into (53), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = F_{2i}. \tag{55}$$

The Equation (55) is the generalized Lagrange equation for the nonconservative system.

2) The generalized Hamilton function for the nonconservative system

When L and w_2 do not include time, the time derivative of $\bar{L}$ is

$$\begin{aligned}\frac{\mathrm{d}\bar{L}}{\mathrm{d}t} &= \frac{\partial L}{\partial q_i}\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i + \frac{\partial w_2}{\partial \boldsymbol{r}} \cdot \frac{\partial \boldsymbol{r}}{\partial q_i}\dot{q}_i\\ &= \frac{\partial L}{\partial q_i}\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i + \boldsymbol{F}_2 \cdot \frac{\partial \boldsymbol{r}}{\partial q_i}\dot{q}_i\\ &= \left(\frac{\partial L}{\partial q_i} + F_{2i}\right)\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i\right),\end{aligned} \tag{56}$$

where $w_2 = \int \boldsymbol{F}_2 \cdot \mathrm{d}\boldsymbol{r}$ and $\boldsymbol{F}_2 = \frac{\partial w_2}{\partial \boldsymbol{r}}$.

With Equation (56), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i-\bar{L}\right)=0, \tag{57}$$

or

$$\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i-L-w_2=\bar{H}=constant, \tag{58}$$

as

$$\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i-L=T+U=H, \tag{59}$$

then

$$\bar{H}=T+U-w_2=H-w_2. \tag{60}$$

The $\bar{H}$ is called the integral of generalized energy, or generalized Hamilton function for the nonconservative force system.

3) The invariance of $\bar{L}$ and the conserved quantity

With Equations (52) and (55), we have

$$\begin{aligned}\delta\bar{L}&=\frac{\partial L}{\partial q_i}\delta q_i+\frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i+F_{2i}\cdot\delta q_i\\&=\left(\frac{\partial L}{\partial q_i}+F_{2i}\right)\delta q_i+\frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i\\&=\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i+\frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i\\&=\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\delta q_i\right)=0.\end{aligned} \tag{61}$$

By the invariance of $\bar{L}$ ($\delta\bar{L}=0$), we can obtain the conserved quantity for the nonconservative system

$$\frac{\partial L}{\partial \dot{q}_i}\delta q_i=constant. \tag{62}$$

It is the same as the conservative system.

6. The Generalized Lagrange Equation and Generalized Hamilton Function for the Heat Exchange System

1) The generalized Lagrange equation for the heat exchange system

In Equation (47), the generalized Lagrange function for the heat exchange system is

$$\bar{L}=T-U-Q=L-Q, \tag{63}$$

In Section 8 (Equation (91)), we have given the microcosmic heat $Q=TS$, the Equation (63) becomes

$$\bar{L}=L-TS. \tag{64}$$

i.e.,

$$\bar{L}=L(q_i,\dot{q}_i,t)-ST(q_i,\dot{q}_i,t), \tag{65}$$

When L and T do not include time, the variation of $\bar{L}$ is

$$\delta\bar{L}=\frac{\partial L}{\partial q_i}\delta q_i+\frac{\partial L}{\partial\dot{q}_i}\delta\dot{q}_i-S\frac{\partial T}{\partial q_i}\delta q_i, \tag{66}$$

substituting Equation (66) into the generalized Hamilton principle (38), there is

$$\begin{aligned}\int_{t_1}^{t_2}\delta\bar{L}\mathrm{d}t&=\int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q_i}\delta q_i+\frac{\partial L}{\partial\dot{q}_i}\delta\dot{q}_i-S\frac{\partial T}{\partial q_i}\delta q_i\right)\mathrm{d}t\\&=\int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q_i}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{q}_i}-S\frac{\partial T}{\partial q_i}\right)\delta q_i\mathrm{d}t=0,\end{aligned} \tag{67}$$

as the δq_i is arbitrary, we obtain

$$\frac{\partial L}{\partial q_i}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{q}_i}-S\frac{\partial T}{\partial q_i}=0 \tag{68}$$

The Equation (68) is the generalized Lagrange equation for the heat exchange system.

2) The generalized Hamilton function for the heat exchange system

When L and T do not include time, the time derivative of $\bar{L}$ is

$$\begin{aligned}\frac{\mathrm{d}\bar{L}}{\mathrm{d}t}&=\frac{\partial L}{\partial q_i}\dot{q}_i+\frac{\partial L}{\partial\dot{q}_i}\ddot{q}_i-S\frac{\partial T}{\partial q_i}\dot{q}_i\\&=\left(\frac{\partial L}{\partial q_i}-S\frac{\partial T}{\partial q_i}\right)\dot{q}_i+\frac{\partial L}{\partial\dot{q}_i}\ddot{q}_i\\&=\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{q}_i}\dot{q}_i+\frac{\partial L}{\partial\dot{q}_i}\ddot{q}_i\\&=\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}_i}\dot{q}_i\right),\end{aligned} \tag{69}$$

With Equation (69), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}_i}\dot{q}_i-\bar{L}\right)=0, \tag{70}$$

or

$$\frac{\partial L}{\partial\dot{q}_i}\dot{q}_i-L+TS=\bar{H}=constant, \tag{71}$$

as

$$\frac{\partial L}{\partial\dot{q}_i}\dot{q}_i-L=T+U=H, \tag{72}$$

then

$$\bar{H}=T+U+Q=H+Q=H+TS. \tag{73}$$

The $\bar{H}$ is called the integral of generalized energy, or generalized Hamilton function for the heat exchange system.

3) The invariance of $\bar{L}$ and the conserved quantity

In Equations (66) and (68), we have

$$\begin{aligned}\delta\bar{L} &= \frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i - S\frac{\partial T}{\partial q_i}\delta q_i \\ &= \left(\frac{\partial L}{\partial q_i} - S\frac{\partial T}{\partial q_i}\right)\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\delta q_i\right) = 0.\end{aligned} \tag{74}$$

By the invariance of $\bar{L}$ ($\delta\bar{L} = 0$), we can obtain the conserved quantity for the heat exchange system

$$\frac{\partial L}{\partial \dot{q}_i}\delta q_i = constant. \tag{75}$$

It is the same as the conservative system.

In the above, we have given the generalized Hamilton principle for the nonconservative force and the heat exchange system. On this basis, we further given the generalized Lagrange function and generalized Hamilton function for the nonconservative force and the heat exchange system. With the results, we shall study the non-Hermitian quantum theory for the nonconservative force and the heat exchange microcosmic system.

7. The Non-Hermitian Quantum Theory for the Nonconservative Force System

With the generalized Hamilton principle and generalized Lagrange function, we will deduce the non-Hermitian quantum theory for the nonconservative force system by the approach of path integral, the path integral formula is

$$\Psi(\boldsymbol{r},t') = \int \exp\left[\frac{i}{\hbar}\int_t^{t'} \bar{L}\left(\dot{\boldsymbol{r}}(\tau),\boldsymbol{r}(\tau),\tau\right)\mathrm{d}\tau\right] D\left[\boldsymbol{r}(t)\right]\Psi(\boldsymbol{r}',t)\,\mathrm{d}\boldsymbol{r}', \tag{76}$$

In Equation (76), the generalized Lagrange function $\bar{L}$ is

$$\bar{L} = T - U + \omega_2 = L + \omega_2 = L + \int \boldsymbol{F}\cdot\mathrm{d}\boldsymbol{r}, \tag{77}$$

where the force $\boldsymbol{F}$ is the nonconservative force, the Equation (76) gives the wave function at a time t' in terms of the wave function at a time *t*. In order to obtain the differential equation, we apply this relationship in the special case that the time t' differs only by an infinitesimal interval ε from *t*. For a short interval ε the action is approximately ε times the Lagrangian for this interval, we have

$$\Psi(\boldsymbol{r},t+\varepsilon) = \int \frac{\mathrm{d}\boldsymbol{r}'}{A^3}\exp\left[\frac{i\varepsilon}{\hbar}\bar{L}\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{\varepsilon},\frac{\boldsymbol{r}+\boldsymbol{r}'}{2},\frac{t'+t}{2}\right)\right]\Psi(\boldsymbol{r}',t), \tag{78}$$

where A is a normalization constant.

Substituting Equation (77) into (78), there is

$$\Psi(\boldsymbol{r},t+\varepsilon) = \int \frac{\mathrm{d}\boldsymbol{r}'}{A^3}\exp\left[\frac{i\varepsilon}{\hbar}\left(\frac{m}{2}\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{\varepsilon}\right)^2 - V\left(\frac{\boldsymbol{r}+\boldsymbol{r}'}{2},\frac{t'+t}{2}\right) + \int_{\boldsymbol{r}'}^{\boldsymbol{r}}\boldsymbol{F}\cdot\mathrm{d}\boldsymbol{r}''\right)\right]\Psi(\boldsymbol{r}',t). \tag{79}$$

In macroscopic field, the frictional force and adhere force are non-conservative force, and the non-conservative force $\boldsymbol{F}$ is directly proportional to velocity $\boldsymbol{v}$, their directions are opposite, *i.e.* $\boldsymbol{F} = -k\boldsymbol{v}$. In microcosmic field, atomic and molecular can also suffer the action of non-conservative force. In the experiment of Bose-Einstein condensates, the atomic Rb^{87}, Na^{23} and Li^{7} can be cooled in laser field, since they get the non-conservative force from the photons.

Substituting $\boldsymbol{F} = -k\boldsymbol{v}$ into Equation (79), we get

$$\begin{aligned}\Psi(\boldsymbol{r}, t+\varepsilon) = \int \frac{\mathrm{d}\boldsymbol{r}'}{A^3} \exp\Bigg[\frac{i\varepsilon}{\hbar}\Bigg(\frac{m}{2}\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{\varepsilon}\right)^2 - V\left(\frac{\boldsymbol{r}+\boldsymbol{r}'}{2}, \frac{t'+t}{2}\right) \\ - k\int_{\boldsymbol{r}'}^{\boldsymbol{r}}\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{\varepsilon}\right)\cdot \mathrm{d}\boldsymbol{r}''\Bigg)\Bigg]\Psi(\boldsymbol{r}', t).\end{aligned} \tag{80}$$

The quantity $\frac{(\boldsymbol{r}-\boldsymbol{r}')^2}{\varepsilon}$ appear in the exponent of the first factor. It is clear that if $\boldsymbol{r}'$ is appreciably different from $\boldsymbol{r}$, this quantity is very large and the exponential consequently oscillates very rapidly as $\boldsymbol{r}'$ varies, when this factor oscillates rapidly, the integral over $\boldsymbol{r}'$ gives a very small value. Only if $\boldsymbol{r}'$ is near $\boldsymbol{r}$ do we get important contributions. For this reason we make the substitution $\boldsymbol{r}' = \boldsymbol{r} + \boldsymbol{\eta}$ with the expectation that appreciable contribution to the integral will occur only for small $\boldsymbol{\eta}$, we obtain

$$\Psi(\boldsymbol{r}, t+\varepsilon) = \int \frac{\mathrm{d}\boldsymbol{\eta}}{A^3} \exp\left[\frac{i\varepsilon}{\hbar}\left(\frac{m}{2}\left(\frac{\boldsymbol{\eta}}{\varepsilon}\right)^2 - V\left(\boldsymbol{r}+\frac{\boldsymbol{\eta}}{2}, t+\frac{\varepsilon}{2}\right) - k\int_{\boldsymbol{r}'}^{\boldsymbol{r}}\frac{-\boldsymbol{\eta}}{\varepsilon}\cdot \mathrm{d}\boldsymbol{r}''\right)\right]\Psi(\boldsymbol{r}+\boldsymbol{\eta}, t) \tag{81}$$

Now we have

$$\int_{\boldsymbol{r}'}^{\boldsymbol{r}} \boldsymbol{\eta}\cdot \mathrm{d}\boldsymbol{r}'' = \int_{\boldsymbol{r}'}^{\boldsymbol{r}} |\boldsymbol{\eta}||\mathrm{d}\boldsymbol{r}''|\cos\theta = |\boldsymbol{\eta}|\int_{\boldsymbol{r}'}^{\boldsymbol{r}} |\mathrm{d}\boldsymbol{r}''|\cos\theta = |\boldsymbol{\eta}|^2 \tag{82}$$

so that

$$k\int_{\boldsymbol{r}'}^{\boldsymbol{r}}\frac{-\boldsymbol{\eta}}{\varepsilon}\cdot \mathrm{d}\boldsymbol{r}'' = -\frac{k}{\varepsilon}|\boldsymbol{\eta}|^2 = -\frac{k}{\varepsilon}\boldsymbol{\eta}^2 \tag{83}$$

substituting Equation (83) into (81), we have

$$\begin{aligned}\Psi(\boldsymbol{r}, t+\varepsilon) &= \int \frac{\mathrm{d}\boldsymbol{\eta}}{A^3} \exp\left[\frac{i\varepsilon}{\hbar}\left(\frac{m}{2}\frac{\boldsymbol{\eta}^2}{\varepsilon^2} - V\left(\boldsymbol{r}+\frac{\boldsymbol{\eta}}{2}, t+\frac{\varepsilon}{2}\right) + \frac{k}{\varepsilon}\boldsymbol{\eta}^2\right)\right]\Psi(\boldsymbol{r}+\boldsymbol{\eta}, t) \\ &= \int \frac{\mathrm{d}\boldsymbol{\eta}}{A^3} \mathrm{e}^{\frac{im\boldsymbol{\eta}^2}{2\hbar\varepsilon}} \mathrm{e}^{-\frac{i\varepsilon}{\hbar}V\left(\boldsymbol{r}+\frac{\boldsymbol{\eta}}{2}, t+\frac{\varepsilon}{2}\right)} \mathrm{e}^{+\frac{i}{\hbar}k\boldsymbol{\eta}^2}\Psi(\boldsymbol{r}+\boldsymbol{\eta}, t)\end{aligned} \tag{84}$$

After more complex calculation, we have

$$i\hbar\frac{\partial\Psi(\boldsymbol{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V - i\hbar\frac{3k}{m}\right)\Psi(\boldsymbol{r}, t) = \hat{H}\Psi(\boldsymbol{r}, t), \tag{85}$$

the Hamiltonian H is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V - i\hbar\frac{3k}{m}. \tag{86}$$

Obviously, the Hamiltonian H is non Hermitian. The Detailed derivation can see the Ref. [21].

8. The Non-Hermitian Quantum Theory for the Thermodynamics

In classical mechanics, the energy of a macroscopic object is

$$E=\frac{p^2}{2m}+V\left(r\right). \tag{87}$$

For a microcosmic particle, when it exchanges heat Q with the outside world, with Equation (48) or (73), the particle total energy should be the sum of kinetic energy, potential energy and thermal energy, it is

$$E=\frac{p^2}{2m}+V\left(r\right)+Q. \tag{88}$$

In thermodynamics, for the infinitely small processes, the entropy is defined as

$$\mathrm{d}S=\frac{\mathrm{d}Q}{T}. \tag{89}$$

For the finite processes, it is

$$Q-Q_0=TS-TS_0. \tag{90}$$

At temperature T, when a particle has the microcosmic entropy S, it should has the thermal potential energy Q, it is

$$Q=TS, \tag{91}$$

the Equation (88) becomes

$$E=\frac{p^2}{2m}+V\left(r\right)+TS. \tag{92}$$

the Equation (92) is the classical total energy of a microcosmic particle. In quantum theory, it should become operator form. it is

$$\hat{H}=\frac{\hat{p}^2}{2m}+\hat{V}\left(r\right)+T\hat{S}. \tag{93}$$

where $\hat{H}=i\hbar\frac{\partial}{\partial t}$, $\hat{p}^2=-\hbar^2\nabla^2$ and $\hat{S}$ is the microcosmic entropy operator.

At the i-th microcosmic state, the classical microcosmic entropy S_{Fi} and S_{Bi} for Fermion and Bose systems are

$$S_{Fi}=-k_B\left[n_i\ln n_i+\left(1-n_i\right)\ln\left(1-n_i\right)\right], \tag{94}$$

and

$$S_{Bi}=-k_B\left[n_i\ln n_i-\left(1+n_i\right)\ln\left(1+n_i\right)\right], \tag{95}$$

where k_B is the Boltzmann constant, n_i is the average particle numbers of particle in the i-th state. For the Fermion (Bose), the $n_i\leq 1$ ($n_i\geq 1$).

In quantum theory, the classical microcosmic entropy should become operator. The microcosmic entropy operator depends on temperature, but it has no the dimension of temperature, and it is non-Hermitian operator because it has to do with heat exchange. So, the microcosmic entropy operator includes the temperature operator $T\frac{\partial}{\partial T}$. Moreover, it has to do with the state distribution. For the Fermion and Bose systems, the microcosmic entropy operator $\hat{S}_{Fi}$ and $\hat{S}_{Bi}$ of a particle in the *i*-th state can be written as

$$\hat{S}_{Fi}=-k_B\left[n_i\ln n_i+\left(1-n_i\right)\ln\left(1-n_i\right)\right]T\frac{\partial}{\partial T}=S_{Fi}T\frac{\partial}{\partial T}, \tag{96}$$

and

$$\hat{S}_{Bi}=-k_B\left[n_i\ln n_i-\left(1+n_i\right)\ln\left(1+n_i\right)\right]T\frac{\partial}{\partial T}=S_{Bi}T\frac{\partial}{\partial T}. \tag{97}$$

We can prove the following operator relation:

$$\hat{T}^{+}=\hat{T}=T, \tag{98}$$

$$\left(-i\frac{\partial}{\partial T}\right)^{+}=-i\frac{\partial}{\partial T} \tag{99}$$

$$\left[\hat{T},\frac{\partial}{\partial T}\right]=-1. \tag{100}$$

With Equations (98) - (100), we find the operator $T\frac{\partial}{\partial T}$ is non-Hermitian, the microcosmic entropy operators (96) and (97) are also non-Hermitian, it leads to the total Hamilton operator (93) is non-Hermitian and space-time inversion (*PT*) symmetry

$$\hat{H}^{+}\neq H,\quad \left(PT\right)H\left(PT\right)^{-1}=H. \tag{101}$$

This is because the particle (atom or molecule) exchanges energy with the external environment, it is an open system, its Hamiltonian operator should be non-Hermitian.

9. The Schroding Equation with Temperature

With the canonical quantization, $E=i\hbar\frac{\partial}{\partial t}$, $\boldsymbol{p}=-i\hbar\nabla$, substituting Equation (96) into (93), we can obtain the Schroding equation with temperature

$$i\hbar\frac{\partial}{\partial t}\psi\left(\boldsymbol{r},t,T\right)=\left(-\frac{\hbar^2}{2m}\nabla^2+V\left(r\right)+\sum_i S_{Fi}T^2\frac{\partial}{\partial T}\right)\psi\left(\boldsymbol{r},t,T\right), \tag{102}$$

By separating variables

$$\psi\left(\boldsymbol{r},t,T\right)=\Psi\left(\boldsymbol{r},T\right)f\left(t\right), \tag{103}$$

we obtain

$$i\hbar\frac{\mathrm{d}f\left(t\right)}{\mathrm{d}t}=E_n f\left(t\right), \tag{104}$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V\left(r\right)+f_nS_{Fi}T^2\frac{\partial}{\partial T}\right)\psi_n\left(\boldsymbol{r},T\right)=E_n\psi_n\left(\boldsymbol{r},T\right). \tag{105}$$

By separating variables $\Psi_n(\boldsymbol{r},T)=\Psi_n(\boldsymbol{r})\phi(T)$, the Equation (105) can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_n(\boldsymbol{r})+V(r)\Psi_n(\boldsymbol{r})=E_{1n}\Psi_n(\boldsymbol{r}), \tag{106}$$

$$f_nS_{Fi}T^2\frac{\partial}{\partial T}\phi(T)=E_{2n}\phi(T) \tag{107}$$

where $E_n=E_{1n}+E_{2n}$, E_{1n} is the eigenenergy obtained by the Schroding Equation (106), E_{2n} is the eigenenergy obtained by the temperature Equation (107), the n expresses the n-th energy level, n_i is the average particle numbers of the i-th state in the n-th energy level, and f_n is the degeneracy of the n-th energy level.

For Equation (107), by the dimensional analysis, the energy E_{2n} can be written as

$$E_{2n}=f_nS_{Fi}T_0=-k_Bf_n\left[n_i\ln n_i+(1-n_i)\ln(1-n_i)\right]T_0, \tag{108}$$

and $\phi(T)$ satisfies equation

$$T^2\frac{\partial}{\partial T}\phi(T)=\phi(T)T_0, \tag{109}$$

the temperature wave function $\phi(T)$ is

$$\phi(T)=A\mathrm{e}^{-\frac{T_0}{T}}, \tag{110}$$

where A is the normalization constant, and T_0 must be the temperature constant, because the energy E_{2n} cannot be the function of variable T, such as the hydrogen atom level is not the function of coordinate variable $\boldsymbol{r}$. The general solution of Equation (102) is

$$\psi(\boldsymbol{r},t,T)=\sum_n C_n\Psi_n(\boldsymbol{r})\phi_n(T)\mathrm{e}^{-\frac{i}{\hbar}E_nt}. \tag{111}$$

For a free particle, its momentum is $\boldsymbol{p}$, and is in the environment of temperature T, because it is in the determinate state, *i.e.*, the average particle numbers $n_i=\delta_{ij}$, the free particle plane wave solution and total energy are

$$\psi(\boldsymbol{r},t,T)=A\mathrm{e}^{\frac{i}{\hbar}\left(\boldsymbol{p}\cdot\boldsymbol{r}-Et+i\frac{T_0}{T}\hbar\right)}, \tag{112}$$

and

$$E=\frac{p^2}{2m}. \tag{113}$$

By the accurate measurement the hydrogen atom spectrum, we can determine the temperature constant T_0. The hydrogen atom has only one electron outside the nucleus, the degeneracy of the n-th energy level is $f_n=n^2$.

When the electron jumps from m-th energy level to the n-th energy level $(m>n)$, the transition frequency without temperature correction (the theoretical calculation with Schroding equation) is

$$\nu_{mn}^{th} = \frac{E_m - E_n}{h}, \tag{114}$$

the transition frequency with temperature correction is

$$\nu_{mn}(T) = \nu_{mn}^{exp} = \frac{E_m(T) - E_n(T)}{h}, \tag{115}$$

the energy levels $E_m(T)$ and $E_n(T)$ are

$$E_m(T) = E_m - k_B f_m \left[m_i \ln m_i + (1-m_i)\ln(1-m_i) \right] T_0, \tag{116}$$

and

$$E_n(T) = E_n - k_B f_n \left[n_i \ln n_i + (1-n_i)\ln(1-n_i) \right] T_0. \tag{117}$$

The average particle numbers of every state in the m-th and n-th energy levels are $m_i = \frac{1}{m^2}$ and $n_i = \frac{1}{n^2}$.

With Equations (114) and (115), we obtain the temperature constant T_0, it is

$$T_0 = \frac{h\left(\nu_{mn}^{exp} - \nu_{mn}^{th}\right)}{k_B \left[\ln \frac{m^2}{n^2} - \left(m^2 - 1\right)\ln\left(1 - \frac{1}{m^2}\right) + \left(n^2 - 1\right)\ln\left(1 - \frac{1}{n^2}\right) \right]}, \tag{118}$$

where h is the Planck constant, by measurement transition frequency ν_{mn}^{exp}, we can determine the temperature constant T_0. When the electron jumps from the first excited state ($m = 2$) to ground state ($n = 1$), the T_0 is

$$T_0 = \frac{h\left(\nu_{21}^{exp} - \nu_{21}^{th}\right)}{k_B \left[4\ln 4 - 3\ln 3\right]}. \tag{119}$$

The theory should be tested by the experiments.

10. Conclusion

The Hamilton principle is a variation principle describing the isolated and conservative systems, its Lagrange function is the difference between kinetic energy and potential energy. By Feynman path integration, we can obtain the standard Schrodinger equation. In this paper, we have given the generalized Hamilton principle, which can describe the heat exchange system, and the nonconservative force system. On this basis, we have further given their generalized Lagrange functions and Hamilton functions. With the Feynman path integration, we have given the generalized Schrodinger equation of nonconservative force system and the heat exchange system.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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