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The generalized Hamilton principle and non-Hermitian quantum theory

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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 Hermitian quantum theory, i.e., the standard Schrodinger equation. In this paper, we have generalized the Hamilton principle to the generalized Hamilton principle, which can describe the open system (mass or energy exchange systems) and nonconservative force systems or dissipative systems, and given the generalized Lagrange function, it has to do with the kinetic energy, potential energy and the work of nonconservative forces to do. With the Feynman path integration, we have given the non-Hermitian quantum theory of the nonconservative force systems. Otherwise, with the generalized Hamilton principle, we have given the generalized Hamiltonian for the particle exchanging heat with the outside world, which is the sum of kinetic energy, potential energy and thermal energy, and further given the equation of quantum thermodynamics.

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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 [4-7]. 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 [10-14], especially those empowered by parity-time symmetry [15]. 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 [16], atomic physics [17], photonics [18], acoustics [19], microwave [20], electronics [21], to quantum information science [22].

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 Hermitian quantum theory, i.e., the standard Schrodinger equation. In this paper, we

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have generalized the Hamilton principle to the generalized Hamilton principle, which can describe the open system (mass or energy exchange systems) and nonconservative force systems or dissipative systems, and given the generalized Lagrange function, it has to do with the kinetic energy, potential energy and the work of nonconservative forces to do. With the Feynman path integration, we have given the non-Hermitian quantum theory of the nonconservative force systems. Otherwise, with the generalized Hamilton principle, we have given the generalized Hamiltonian for the particle exchanging heat with the outside world, which is the sum of kinetic energy, potential energy and thermal energy, and further given the equation of quantum thermodynamics.

2. The generalized Hamilton principle

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

$$f(\vec{r}_i, \dot{\vec{r}}_i, t) = 0, \quad (i = 1, 2, \dots, h) \quad (1)$$

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 $q_1, q_2, \dots, q_{3N-h}$, the position vector $\vec{r}_i$ can be written as

$$\vec{r}_i = \vec{r}_i(q_1, q_2, \dots, q_{3N-h}, t), \quad (i = 1, 2, \dots, N) \quad (2)$$

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

$$\vec{q} = [q_1, q_2, \dots, q_{3N-h}], \quad (3)$$

the virtual displacement are

$$\delta \vec{q} = [\delta q_1, \delta q_2, \dots, \delta q_{3N-h}], \quad (4)$$

the generalized velocity is

$$\dot{\vec{q}} = \frac{d\vec{q}}{dt} = [\dot{q}_1, \dot{q}_2, \dots, \dot{q}_{3N-h}], \quad (5)$$

where $\dot{q}_i = \frac{dq_i}{dt}$.
with Eq. (2), we have

$$\delta \vec{r}_i = \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j, \quad (6)$$

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

$$\delta \omega = \sum_i^N \vec{F}_i \cdot \delta \vec{r}_i = \sum_i \vec{F}_i \cdot \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j = \sum_j (\sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j}) \delta q_j = \sum_j Q_j \delta q_j, \quad (7)$$

the generalized force Q_j is

$$Q_j = \sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j}, \quad (8)$$

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

$$\delta \omega = \sum_j Q_j \delta q_j = -\delta U, \quad (9)$$

where U is the potential energy.

In rectangular coordinates, there is

$$\vec{F} = -\nabla U, \quad (10)$$

and the component is

$$F_i = -\frac{\partial U}{\partial x}. \quad (11)$$

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

$$\int_{t_1}^{t_2} T dt = \int_{t_1}^{t_2} T(q_i, \dot{q}_i, t) dt, \quad (12)$$

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

The variation of Eq. (12) is

$$\delta \int_{t_1}^{t_2} T dt = \int_{t_1}^{t_2} \delta T dt = \int_{t_1}^{t_2} \sum_i m_i \vec{v}_i \cdot \delta \vec{v}_i dt, \quad (13)$$

with $\vec{v}_i = \frac{d\vec{r}_i}{dt}$, we have

$$\delta \vec{v}_i = \frac{d(\delta \vec{r}_i)}{dt} \quad (14)$$

the Eq. (13) becomes

$$\delta \int_{t_1}^{t_2} T dt = \int_{t_1}^{t_2} \sum_i m_i \vec{v}_i \cdot \frac{d(\delta \vec{r}_i)}{dt} dt = \sum_i m_i \vec{v}_i \cdot \delta \vec{r}_i \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \sum_i m_i \dot{\vec{v}}_i \cdot \delta \vec{r}_i dt \quad (15)$$

i.e.,

$$\delta \int_{t_1}^{t_2} T dt + \int_{t_1}^{t_2} \sum_i m_i \dot{\vec{v}}_i \cdot \delta \vec{r}_i dt = \sum_i m_i \dot{\vec{v}}_i \cdot \delta \vec{r}_i \Big|_{t_1}^{t_2} \quad (16)$$

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

$$\delta \int_{t_1}^{t_2} T dt + \int_{t_1}^{t_2} \sum_i \vec{F}_i \cdot \delta \vec{r}_i dt = \sum_i m_i \dot{\vec{v}}_i \cdot \delta \vec{r}_i \Big|_{t_1}^{t_2} \quad (17)$$

and

$$\delta \int_{t_1}^{t_2} T dt + \int_{t_1}^{t_2} \delta \omega dt = \sum_i m_i \dot{\vec{v}}_i \cdot \delta \vec{r}_i \Big|_{t_1}^{t_2}, \quad (18)$$

if the variation of two endpoints are zero, there are

$$\delta q_j \Big|_{t_1} = \delta q_j \Big|_{t_2} = 0 \quad (19)$$

and

$$\delta \vec{r}_i \Big|_{t_1} = \delta \vec{r}_i \Big|_{t_2} = 0 \quad (20)$$

the Eq. (18) becomes

$$\delta \int_{t_1}^{t_2} T dt + \int_{t_1}^{t_2} \delta \omega dt = 0, \quad (21)$$

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

$$\delta \int_{t_1}^{t_2} T dt = \int_{t_1}^{t_2} \delta T dt. \quad (22)$$

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

$$\int_{t_1}^{t_2} \vec{F} \cdot \delta \vec{r} dt = \int_{t_1}^{t_2} \delta \omega dt = - \int_{t_1}^{t_2} \delta U dt = - \delta \int_{t_1}^{t_2} U dt, \quad (23)$$

the Eq. (21) becomes

$$\delta \int_{t_1}^{t_2} (T - U) dt = 0, \quad (24)$$

i.e.,

$$\delta \int_{t_1}^{t_2} L dt = 0. \quad (25)$$

Where the Lagrange function $L = T - V$. The Eq. (25) is the Hamilton principle.

(2) When the active forces are both conservative force F_1 and nonconservative force F_2 , we have

$$\delta \omega = \vec{F}_1 \cdot \delta \vec{r} + \vec{F}_2 \cdot \delta \vec{r} = \delta \omega_1 + \delta \omega_2, \quad (26)$$

and

$$\int_{t_1}^{t_2} \vec{F}_1 \cdot \delta \vec{r} dt = \int_{t_1}^{t_2} \delta \omega_1 dt = - \int_{t_1}^{t_2} \delta U dt = - \delta \int_{t_1}^{t_2} U dt, \quad (27)$$

substituting Eqs. (26) and (27) into (21), there are

$$\delta \int_{t_1}^{t_2} (T - U) dt + \int_{t_1}^{t_2} \delta \omega_2 dt = 0, \quad (28)$$

and

$$\int_{t_1}^{t_2} \delta (T - U) dt + \int_{t_1}^{t_2} \delta \omega_2 dt = 0, \quad (29)$$

or

$$\int_{t_1}^{t_2} \delta (T - U + \omega_2) dt = 0, \quad (30)$$

we define generalized Lagrange function

$$\bar{L} = T - U + \omega_2 = L + \omega_2, \quad (31)$$

the Eq. (30) becomes

$$\int_{t_1}^{t_2} \delta \bar{L} dt = \int_{t_1}^{t_2} \delta(L + \omega_2) dt = 0. \quad (32)$$

The Eq. (32) is called the generalized Hamilton principle, which is different from the Hamilton principle (25), it contains the work of nonconservative force, and the variation is inside the integral sign.

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

$$\delta \omega_2 = \sum_{i=1}^N \vec{F}_{2i} \cdot \delta \vec{r}_i = \sum_j \left(\sum_i \vec{F}_{2i} \cdot \frac{\partial \vec{r}_i}{\partial q_j} \right) \delta q_j = \sum_i \left(\sum_{j=1}^N \vec{F}_{2j} \cdot \frac{\partial \vec{r}_j}{\partial q_i} \right) \delta q_i. \quad (33)$$

For a single nonconservative force F_2 , there is

$$\delta \omega_2 = \sum_i \vec{F}_2 \cdot \frac{\partial \vec{r}}{\partial q_i} \delta q_i, \quad (34)$$

substituting Eq. (34) into (32), there is

$$\int_{t_1}^{t_2} \bar{L} dt = \int_{t_1}^{t_2} \left[\frac{\partial \bar{L}}{\partial q_i} \delta q_i + \frac{\partial \bar{L}}{\partial \dot{q}_i} \delta \dot{q}_i + \vec{F}_2 \cdot \frac{\partial \vec{r}}{\partial q_i} \delta q_i \right] dt = \int_{t_1}^{t_2} \left[\frac{\partial \bar{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \bar{L}}{\partial \dot{q}_i} + \vec{F}_2 \cdot \frac{\partial \vec{r}}{\partial q_i} \right] \delta q_i dt = 0, \quad (35)$$

the variation δq_i is arbitrary, we get

$$\frac{d}{dt} \frac{\partial \bar{L}}{\partial \dot{q}_i} - \frac{\partial \bar{L}}{\partial q_i} = F_{2i}. \quad (36)$$

When a particle are both conservative force F_1 and nonconservative force F_2 , the generalized Lagrange function is

$$\bar{L} = T - U + \omega_2 = L + \int \vec{F}_2 \cdot d\vec{r}, \quad (37)$$

the generalized action is

$$\bar{S} = \int_0^t \bar{L} dt. \quad (38)$$

In the mechanical, the change rate of energy is

$$\frac{dE}{dt} = \vec{F} \cdot \vec{v}. \quad (39)$$

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

$$\frac{dE}{dt} = \frac{dQ}{dt}, \quad (40)$$

and the radiant force should be produced, it is

$$\vec{F} \cdot \vec{v} = \frac{dQ}{dt}, \quad (41)$$

when the microcosmic particle absorb heat, $\frac{dQ}{dt} > 0$, the radiant force is $\vec{F} = -k\vec{v}$. When the microcosmic particle deliver heat, $\frac{dQ}{dt} < 0$, the radiant force is $\vec{F} = k\vec{v}$. The Eq. (41) should be changed to the following formula

$$\vec{F} \cdot \vec{v} = -\frac{dQ}{dt}, \quad (42)$$

i.e.,

$$\vec{F} \cdot d\vec{r} = \vec{F} \cdot \vec{v} dt = -dQ, \quad (43)$$

then

$$\int \vec{F} \cdot d\vec{r} = - \int dQ = -Q, \quad (44)$$

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

$$\bar{L} = T - U + \int \vec{F} \cdot d\vec{r} = L - Q \quad (45)$$

and the generalized Hamiltonian function is

$$\bar{H} = p\dot{q} - \bar{L} = T + U + Q. \quad (46)$$

3. The non-Hermitian quantum theory for the nonconservative force system

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

$$\Psi(\vec{r}, t') = \int \exp\left[\frac{i}{\hbar} \int_t^{t'} \bar{L}(\vec{r}(\tau), \dot{\vec{r}}(\tau), \tau) d\tau\right] D[\vec{r}(t)] \Psi(\vec{r}', t) d\vec{r}', \quad (47)$$

gives the wave function at a time t_2 in terms of the wave function at a time t_1 . In order to obtain the differential equation, we apply this relationship in the special case that the time t_2 differs only by an infinitesimal interval ε from t_1 . For a short interval ε the action is approximately ε times the Lagrangian for this interval, we have

$$\Psi(\vec{r}, t + \varepsilon) = \int \frac{d\vec{r}'}{A^3} \exp\left[\frac{i\varepsilon}{\hbar} \bar{L}\left(\frac{\vec{r} - \vec{r}'}{\varepsilon}, \frac{\vec{r} + \vec{r}'}{2}, \frac{t' + t}{2}\right)\right] \Psi(\vec{r}', t), \quad (48)$$

where A is a normalization constant. Substituting Eq. (37) into (46), there is

$$\Psi(\vec{r}, t + \varepsilon) = \int \frac{d\vec{r}'}{A^3} \exp\left[\frac{i\varepsilon}{\hbar} \left(\frac{m}{2} \left(\frac{\vec{r} - \vec{r}'}{\varepsilon}\right)^2 - V\left(\frac{\vec{r} + \vec{r}'}{2}, \frac{t' + t}{2}\right) + \int_{\vec{r}'}^{\vec{r}} \vec{F} \cdot d\vec{r}''\right)\right] \Psi(\vec{r}', t). \quad (49)$$

In macroscopic field, the frictional force and adhere force are non-conservative force, and the non-conservative force $\vec{F}$ is directly proportional to velocity $\vec{v}$, their directions are opposite, i.e. $\vec{F} = -k\vec{v}$. 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 $\vec{F} = -k\vec{v}$ into Eq. (47), we get

$$\begin{aligned} \Psi(\vec{r}, t + \varepsilon) = & \int \frac{d\vec{r}'}{A^3} \exp\left[\frac{i\varepsilon}{\hbar} \left(\frac{m}{2} \left(\frac{\vec{r} - \vec{r}'}{\varepsilon}\right)^2 - V\left(\frac{\vec{r} + \vec{r}'}{2}, \frac{t' + t}{2}\right) \right. \right. \\ & \left. \left. - k \int_{\vec{r}'}^{\vec{r}} \left(\frac{\vec{r} - \vec{r}'}{\varepsilon}\right) \cdot d\vec{r}''\right)\right] \Psi(\vec{r}', t). \end{aligned} \quad (50)$$

The quantity $\frac{(\vec{r} - \vec{r}')^2}{\varepsilon}$ appear in the exponent of the first factor. It is clear that if $\vec{r}'$ is appreciably different from $\vec{r}$, this quantity is very large and the exponential consequently oscillates very rapidly as $\vec{r}'$ varies, when this factor oscillates rapidly, the integral over $\vec{r}'$ gives a very small value. Only if $\vec{r}'$ is near $\vec{r}$ do we

get important contributions. For this reason we make the substitution $\vec{r}' = \vec{r} + \vec{\eta}$ with the expectation that appreciable contribution to the integral will occur only for small $\vec{\eta}$, we obtain

$$\Psi(\vec{r}, t + \varepsilon) = \int \frac{d\vec{\eta}}{A^3} \exp\left[\frac{i\varepsilon}{\hbar} \left(\frac{m}{2} \left(\frac{\vec{\eta}}{\varepsilon}\right)^2 - V\left(\vec{r} + \frac{\vec{\eta}}{2}, t + \frac{\varepsilon}{2}\right) - k \int_{\vec{r}'}^{\vec{r}} \frac{-\vec{\eta}}{\varepsilon} \cdot d\vec{r}''\right)\right] \Psi(\vec{r} + \vec{\eta}, t) \quad (51)$$

Now we have

$$\int_{\vec{r}'}^{\vec{r}} \vec{\eta} \cdot d\vec{r}'' = \int_{\vec{r}'}^{\vec{r}} |\vec{\eta}| |d\vec{r}''| \cos \theta = |\vec{\eta}| \int_{\vec{r}'}^{\vec{r}} |d\vec{r}''| \cos \theta = |\vec{\eta}|^2 \quad (52)$$

so that

$$k \int_{\vec{r}'}^{\vec{r}} \frac{-\vec{\eta}}{\varepsilon} \cdot d\vec{r}'' = -\frac{k}{\varepsilon} |\vec{\eta}|^2 = -\frac{k}{\varepsilon} \vec{\eta}^2 \quad (53)$$

substituting Eq. (51) into (49), we have

$$\begin{aligned} \Psi(\vec{r}, t + \varepsilon) &= \int \frac{d\vec{\eta}}{A^3} \exp\left[\frac{i\varepsilon}{\hbar} \left(\frac{m}{2} \frac{\vec{\eta}^2}{\varepsilon^2} - V\left(\vec{r} + \frac{\vec{\eta}}{2}, t + \frac{\varepsilon}{2}\right) + \frac{k}{\varepsilon} \vec{\eta}^2\right)\right] \Psi(\vec{r} + \vec{\eta}, t) \\ &= \int \frac{d\vec{\eta}}{A^3} e^{\frac{im\vec{\eta}^2}{2\hbar\varepsilon}} e^{-\frac{i\varepsilon}{\hbar} V\left(\vec{r} + \frac{\vec{\eta}}{2}, t + \frac{\varepsilon}{2}\right)} e^{\frac{k}{\hbar} \vec{\eta}^2} \Psi(\vec{r} + \vec{\eta}, t) \end{aligned} \quad (54)$$

After more complex calculation, we have

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V - i\hbar \frac{3k}{m}\right) \Psi(\vec{r}, t) = \hat{H} \Psi(\vec{r}, t), \quad (55)$$

the Hamiltonian H is

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V - i\hbar \frac{3k}{m}. \quad (56)$$

Obviously, the Hamiltonian H is non Hermitian. The Detailed derivation can see the Ref. [23]

4. The non-Hermitian quantum theory for the thermodynamics

In classical mechanics, the energy of a macroscopic object is

$$E = \frac{p^2}{2m} + V(r). \quad (57)$$

For a microcosmic particle, when it exchanges heat Q with the outside world, with Eq. (46), the particle total energy should be the sum of kinetic energy, potential energy and thermal energy, it is

$$E = \frac{p^2}{2m} + V(r) + Q. \quad (58)$$

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

$$dS = \frac{dQ}{T}. \quad (59)$$

For the finite processes, it is

$$Q - Q_0 = TS - TS_0. \quad (60)$$

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

$$Q = TS, \quad (61)$$

the Eq. (58) becomes

$$E = \frac{p^2}{2m} + V(r) + TS. \quad (62)$$

the Eq. (62) is the classical total energy of a microcosmic particle. In quantum theory, it should become operator form. it is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(r) + T\hat{S}. \quad (63)$$

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_i^F and S_i^B for Fermion and Bose systems are

$$S_i^F = -k_B [n_i \ln n_i + (1 - n_i) \ln(1 - n_i)], \quad (64)$$

and

$$S_i^B = -k_B [n_i \ln n_i - (1 + n_i) \ln(1 + n_i)], \quad (65)$$

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

In quantum theory, the classical microcosmic entropy should become operator. Obviously, the microcosmic entropy operator depends on temperature, and it is dimensionless and non-Hermitian (heat exchange), the microcosmic entropy operator should include the temperature operator $T \frac{\partial}{\partial T}$. Moreover, it has to do with state. The microcosmic entropy operator $\hat{S}_i^F$ and $\hat{S}_i^B$ of a particle in the i -th state for Fermion and Bose systems can be defined as

$$\hat{S}_i^F = -k_B [n_i \ln n_i + (1 - n_i) \ln(1 - n_i)] T \frac{\partial}{\partial T} = S_{Fi} T \frac{\partial}{\partial T}, \quad (66)$$

and

$$\hat{S}_i^B = -k_B [n_i \ln n_i - (1 + n_i) \ln(1 + n_i)] T \frac{\partial}{\partial T} = S_{Bi} T \frac{\partial}{\partial T}. \quad (67)$$

Where $S_{Fi} = -k_B [n_i \ln n_i + (1 - n_i) \ln(1 - n_i)]$ and $S_{Bi} = -k_B [n_i \ln n_i - (1 + n_i) \ln(1 + n_i)]$.

We can prove the following operator relation:

$$\hat{T}^+ = \hat{T} = T, \quad (68)$$

$$(-i \frac{\partial}{\partial T})^+ = -i \frac{\partial}{\partial T} \quad (69)$$

$$[\hat{T}, \frac{\partial}{\partial T}] = -1. \quad (70)$$

With Eqs. (68)-(70), we can prove the operator $T \frac{\partial}{\partial T}$ is non-Hermitian operator, and the microcosmic entropy operators (66) and (67) are non-Hermitian operator, it leads to the Hamilton operator H is non-Hermitian and PT symmetrical, there are

$$\hat{H}^+ \neq H, \quad (PT)H(PT)^{-1} = H. \quad (71)$$

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

5. The Schrodinger equation with temperature

With the canonical quantization, $E = i\hbar \frac{\partial}{\partial t}$, $\vec{p} = -i\hbar \nabla$, substituting Eq. (66) into (63), we can obtain the Schrodinger equation with temperature

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t, T) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) + \sum_i S_{Fi} T^2 \frac{\partial}{\partial T} \right) \psi(\vec{r}, t, T), \quad (72)$$

By separating variables

$$\psi(\vec{r}, t, T) = \Psi(\vec{r}, T) f(t), \quad (73)$$

we obtain

$$i\hbar \frac{df(t)}{dt} = E_n f(t), \quad (74)$$

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) + f_n S_{Fi} T^2 \frac{\partial}{\partial T} \right) \psi_n(\vec{r}, T) = E_n \psi_n(\vec{r}, T). \quad (75)$$

By separating variables $\Psi_n(\vec{r}, T) = \Psi_n(\vec{r}) \phi(T)$, the Eq. (75) can be written as

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi_n(\vec{r}) + V(r) \Psi_n(\vec{r}) = E_{1n} \Psi_n(\vec{r}), \quad (76)$$

$$f_n S_{Fi} T^2 \frac{\partial}{\partial T} \phi(T) = E_{2n} \phi(T) \quad (77)$$

where $E_n = E_{1n} + E_{2n}$, E_{1n} is the eigenenergy obtained by the Schrodinger equation (76), E_{2n} is the eigenenergy obtained by the temperature equation (77), 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.

From Eq. (77), we can obtain its solution

$$E_{2n} = f_n S_{Fi} T_0 = -k_B f_n [n_i \ln n_i + (1 - n_i) \ln(1 - n_i)] T_0, \quad (78)$$

and

$$T^2 \frac{\partial}{\partial T} \phi(T) = \phi(T) T_0, \quad (79)$$

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

$$\phi(T) = A e^{-\frac{T_0}{T}}, \quad (80)$$

where A is the normalization constant, and T_0 is the temperature constant. The general solution of Eq. (72) is

$$\psi(\vec{r}, t, T) = \sum_n C_n \Psi_n(\vec{r}) \phi_n(T) e^{-\frac{i}{\hbar} E_n t}. \quad (81)$$

For a free particle, its momentum is $\vec{p}$, 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

$$\psi(\vec{r}, t, T) = A e^{\frac{i}{\hbar} (\vec{p} \cdot \vec{r} - E t + i \frac{T_0}{T} \hbar)}, \quad (82)$$

and

$$E = \frac{p^2}{2m}. \quad (83)$$

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 Schrodinger equation) is

$$\nu_{mn}^{th} = \frac{E_m - E_n}{h}, \quad (84)$$

the transition frequency with temperature correction is

$$\nu_{mn}(T) = \nu_{mn}^{exp} = \frac{E_m(T) - E_n(T)}{h}, \quad (85)$$

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

$$E_m(T) = E_m - k_B f_m [m_i \ln m_i + (1 - m_i) \ln(1 - m_i)] T_0, \quad (86)$$

and

$$E_n(T) = E_n - k_B f_n [n_i \ln n_i + (1 - n_i) \ln(1 - n_i)] T_0. \quad (87)$$

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 Eqs. (84) and (85), we obtain the temperature constant T_0 , it is

$$T_0 = \frac{h(\nu_{mn}^{exp} - \nu_{mn}^{th})}{k_B [\ln \frac{m^2}{n^2} - (m^2 - 1) \ln(1 - \frac{1}{m^2}) + (n^2 - 1) \ln(1 - \frac{1}{n^2})]}, \quad (88)$$

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

$$T_0 = \frac{h(\nu_{21}^{exp} - \nu_{21}^{th})}{k_B [4 \ln 4 - 3 \ln 3]}. \quad (89)$$

The theory should be tested by the future experiments.

6. Conclusions

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 Hermitian quantum theory, i.e., the standard Schrodinger equation. In this paper, we have generalized the Hamilton principle to the generalized Hamilton principle, which can describe the open system (mass or energy exchange systems) and nonconservative force systems or dissipative systems, and given the generalized Lagrange function, it has to do with the kinetic energy, potential energy and the work of nonconservative forces to do. With the Feynman path integration, we have given the non-Hermitian quantum theory of the nonconservative force systems. Otherwise, with the generalized Hamilton principle, we have given the generalized Hamiltonian for the particle exchanging heat with the outside world, which is the sum of kinetic energy, potential energy and thermal energy, and further given the equation of quantum thermodynamics.

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