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Research Article

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The non-relativistic and relativistic quantum theory with temperature

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Abstract
In this paper, we have proposed the non-Hermitian theory of quantum thermodynamics, and given the quantum thermodynamics equations, including non-relativistic and relativistic quantum theory with temperature, i.e., the temperature-dependent schrodinger equation, Dirac equation and photon equation. We give the solution of wave function and energy level with temperature, and introduced the temperature constant T0, which should be determined by the atom or molecule spectrum experiments. PACS: 03.65.-w, 05.70.Ce, 05.30.Rt.

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Introduction
The study of the physical properties of materials, focusing on its thermodynamic properties, is of great interest in condensed matter physics, solid-state physics, and materials science [1, 2]. The classical thermodynamics is built with the concept of equilibrium states. However, it is less clear how equilibrium thermodynamics emerges through the dynamics that follows the principle of quantum mechanics. The behaviour of quantum many-body systems driven out-of-equilibrium is one of the grand challenges of modern physics. The problem is particularly challenging when treating the dynamics of realistic finite-temperature systems, rather than systems evolving from the zero-temperature ground state. Recent development in the field of quantum thermodynamics taking place under nonequilibrium state [3-7]. The quantum thermodynamics which has grown rapidly over the last decade. It is fuelled by recent equilibration experiments [8] in cold atomic and other physical systems, the introduction of new numerical methods [9], and the discovery of fundamental theoretical relationships in non-equilibrium statistical physics and quantum information theory [10-13]. In this paper, we have proposed the non-Hermitian theory of quantum thermodynamics, and given the quantum thermodynamics equations, including non-relativistic and relativistic quantum theory, i.e., the temperature-dependent schrodinger equation, Dirac equation and photon equation. We give the solution of wave function and energy level with temperature, and introduced the temperature constant T0, which should be determined by the atom or molecule spectrum experiments.

The principle of quantum thermodynamics
In classical mechanics, the energy of a particle is

$$E = \frac{p^2}{2m} + V(r), \quad (1)$$

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

$$dS = \frac{dQ}{T}. \quad (2)$$

For the finite processes, it is

$$Q - Q_0 = TS - TS_0. \quad (3)$$

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

$$Q = TS. \quad (4)$$

If there is an heat quantity exchange between the particle and the external environment, the total energy of particle should be the sum of kinetic energy, potential energy and thermal potential energy, it is

$$E = \frac{p^2}{2m} + V(r) + Q = \frac{p^2}{2m} + V(r) + TS. \quad (5)$$

Where $p^2 / 2m$ is the particle kinetic energy, V (r) is the potential energy, TS is called the particle thermal potential energy, T is the temperature of particle in the external environment, and S is the particle microcosmic entropy. The Eq. (5) is the classical total energy of particle, it should become operator form in quantum theory, it is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(r) + T\hat{S}. \quad (6)$$

Where Hˆ = i~∂t∂ , ˆp2 = −~²∇² and Sˆ is the microcosmic entropy operator of a particle.
At the i − th microcosmic state, the classical microcosmic entropy and for Fermion and Bose systems are

$$S_i^F = -kB[n_i \ln n_i + (1 - n_i)\ln(1 - n_i)], \quad (7)$$

and

$$S_i^B = -k_B[n_i \ln n_i - (1 + n_i)\ln(1 + n_i)], \quad (8)$$

where k_B is the Boltzmann constant, ni 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 quantum microcosmic entropy should become quantum operator. The microcosmic entropy operator $\hat{S}_i^F$. $\hat{S}_i^B$and of a particle in the i − th state for Fermion and Bose systems are

$$\hat{S}_i^F = -k_B[n_i \ln n_i + (1 - n_i)\ln(1 - n_i)]T\frac{\partial}{\partial T} = S_{Fi}T\frac{\partial}{\partial T}. \quad (9)$$

and

$$\hat{S}_i^B = -k_B[n_i \ln n_i - (1 + n_i)\ln(1 + n_i)]T\frac{\partial}{\partial T} = S_{Bi}T\frac{\partial}{\partial T}. \quad (10)$$

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

The microcosmic entropy operator should contain temperature, and it is dimensionless, the microcosmic entropy operators (9) and (10) can be obtained by adding temperature operator T ∂T∂ to classical microcosmic entropy (7) and (8).
We can prove the following operator relation:

$$\hat{T}^+ = \hat{T} = T, \quad (11)$$

$$(-i\frac{\partial}{\partial T})^+ = -i\frac{\partial}{\partial T} \quad (12)$$

$$[\hat{T}, \frac{\partial}{\partial T}] = -1. \quad (13)$$

With Eqs. (11)-(13), we can prove the operator T ∂T∂ is not Hermitian operator, i.e., the microcosmic entropy operators (9) and (10) are not Hermitian operator, but their Hamilton operator H is PT symmetrical, there are

$$\hat{H}^+ \neq H, \quad (PT)H(PT)^{-1} = H. \quad (14)$$

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

The Schroding equation with temperature

With the canonical quantization, $E = i\hbar\partial_t$, $\vec{p} = -i\hbar\nabla$, substituting Eq. (9) into (6), we can obtain the Schroding equation with temperature

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t, T) = (-\frac{\hbar^2}{2m}\nabla^2 + V(r) + S_{Fi}T^2\frac{\partial}{\partial T})\psi(\vec{r}, t, T). \quad (15)$$

By separating variables

$$\psi(\vec{r}, t, T) = \Psi(\vec{r}) f(t)\varphi(T), \quad (16)$$

we obtain

$$i\hbar\frac{df(t)}{dt} = E_n f(t), \quad (17)$$

$$(-\frac{\hbar^2}{2m}\nabla^2 + V(r) + S_{Fi}T^2\frac{\partial}{\partial T})\psi_n(\vec{r}, T) = E_n\psi_n(\vec{r}, T), \quad (18)$$

the Eq. (18) can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_n(\vec{r}) + V(r)\Psi_n(\vec{r}) = E_{1n}\Psi_n(\vec{r}), \quad (19)$$

$$f_n S_{Fi}T^2\frac{\partial}{\partial T}\phi(T) = E_{2n}\phi(T) \quad (20)$$

where $E_n = E_{1n} + E_{2n}$, $E1_n$ is the eigenenergy obtained by the Schroding equation (19), E_{2n} is the eigenenergy obtained by the temperature equation (20), n expresses the n−th energy level, ni is the average particle numbers of the $i - th$ state in the $n - th$ energy level, and fn is the degeneracy of the $n - th$ energy level.

From Eq. (20), we can obtain its solution

$$E_{2n} = \text{SFiT0} \quad (21)$$

and

$$T^2\frac{\partial}{\partial T}\phi(T) = \phi(T)T_0, \quad (22)$$

the solution of temperature wave function is

$$\phi(T) = Ae^{-\frac{T_0}{T}}. \quad (23)$$

Where A is the normalization constant, and T_0 is the temperature constant. The general solution of Eq. (15) is

$$\psi(\vec{r}, t, T) = \sum C_n\Psi_n(\vec{r})\phi_n(T)e^{-\frac{i}{\hbar}E_n t} \quad (24)$$

For the free particle of momentum $\vec{p}$, and in a temperature T environment, its plane wave solution and total energy are

$$\psi(\vec{r},t,T) = Ae^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-Et+i\frac{T_0}{T}\hbar)}, \tag{25}$$

$$E = \frac{p^2}{2m.} \tag{26}$$

By the accurate measurement atom spectrum, we can determine the temperature constant T0, the transition frequency without temperature correction (the theoretical calculation with Schroding equation) is

$$\nu_{mn}^{th} = \frac{E_m - E_n}{h}, \tag{27}$$

the transition frequency with temperature correction (the experiment measurement) is

$$\nu_{mn}^{exp} = \frac{E_m(T) - E_n}{h} = \frac{E_m - k_B T_0 2\ln 2 - E_n}{h} = \nu_{mn}^{th} - \frac{2k_B T_0 \ln 2}{h}, \tag{28}$$

with Eqs. (28) and (29), we obtain

$$T_o = \frac{h(\nu_{mn}^{th} - \nu_{mn}^{exp})}{2k_B \ln 2}. \tag{29}$$

Where h is the Planck constant, by measurement transition frequency v_{mn}^{exp}, we can determine the temperature constant T_0.

The Dirac equation with temperature

In section 3, we have studied the quantum theory with temperature for the low energy non-relativistic particle. In the following, we should consider the high energy relativistic case. As is known to all, Dirac equation describes the particle of spin , such as electron, by factorizing Einstein's dispersion relation, such that the field equation becomes the first order in time derivative [16]. Namely, Dirac factorized the relativistic dispersion relation employing four by four matrices, which is expressed as

$$E^2 - c^2p\sim{}^2 - m^2{}_0c^4 = \tag{30}$$

$$(E - cp\sim\cdot\alpha\sim - m_0c^2\beta)(E + cp\sim\cdot\alpha\sim + m_0c^2\beta) = 0,$$

thus we get

$$E - c\alpha\sim\cdot p\sim - m_0c^2\beta = 0. \tag{31}$$

By canonical quantization Eq. (32), i.e., $E \rightarrow$ i~∂t$^{\partial}$, $p\sim \rightarrow -i\sim\nabla$, we can obtain the Dirac spinor wave equation

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = (-ic\hbar\vec{\alpha}\cdot\vec{\nabla} + m_0c^2\beta)\psi(\vec{r},t), \tag{32}$$

where α~ and β are Dirac matrices, and $\psi(\sim r,t)$ is spinor wave function, they are

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & i \end{pmatrix}, \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{33}$$

and

$$\psi(\vec{r},t) = \begin{pmatrix} \psi_1(\vec{r},t) \\ \psi_2(\vec{r},t) \\ \psi_3(\vec{r},t) \\ \psi_4(\vec{r},t) \end{pmatrix} \tag{34}$$

When the particle of spin 1/2 is in temperature T external environment, we should consider the thermal potential energy $Q = TS$, the Eq. (31) should be written as

$$(E - TS - V(r))^2 - c^2p\sim{}^2 - m^2{}_0c^4 = \tag{37}$$

$$(E - TS - V(r) - cp\sim\cdot\alpha\sim - m_0c^2\beta)(E - TS - V(r) + cp\sim\cdot\alpha\sim + m_0c^2\beta) = 0,$$

where $V(r)$ is the particle potential energy. it is similar to Eq. (33), we obtain the Dirac equation with temperature, it is

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t,T) = (T\hat{S} + V(r) - ic\hbar\vec{\alpha}\cdot\vec{\nabla} + m_0c^2\beta)\psi(\vec{r},t,T), \tag{38}$$

substituting Eq. (8) into (39), we obtain

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t,T) = (-k_Bn_i\ln n_iT^2\frac{\partial}{\partial T} + V(r) - ic\hbar\vec{\alpha}\cdot\vec{\nabla} + m_0c^2\beta)\psi(\vec{r},t,T), \tag{39}$$

The eigen equation of Eq. (40) is

$$(-k_Bn_i\ln n_iT^2\frac{\partial}{\partial T} + V(r) - ic\hbar\vec{\alpha}\cdot\vec{\nabla} + m_0c^2\beta)\psi_n(\vec{r},T) = E_n\psi_n(\vec{r},T), \tag{40}$$

by separating variables

$$\psi(\sim r,T) = \psi_n(\sim r)\varphi(T), \tag{41}$$

we obtain

$$(-ic\sim\alpha\sim\cdot 5\sim + V(r) + m_0c^2\beta)\psi_n(\sim r) = E_{1n}\psi_n(\sim r), \tag{42}$$

$$-k_Bn_i\ln n_iT^2\frac{\partial}{\partial T}\phi(T) = E_{2n}\phi(T), \tag{43}$$

the total energy level is

$$E = E1n - kBT0ni\ \ln ni. \tag{44}$$

The photon quantum theory with and without temperature

With Dirac's factorization approach, we can obtain the spinor wave equation of free photon. For a photon, its mass $m_0 = 0$, Eq. (31) becomes

$$E - c\alpha\sim p\sim = 0. \tag{45}$$

By canonical quantization Eq. (45), we obtain the spinor wave equation of photon

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = -ic\hbar\vec{\alpha}\cdot\vec{\nabla}\psi(\vec{r},t) = H\psi(\vec{r},t), \tag{46}$$

where $H = -ic\sim\alpha\sim\cdot 5\sim$ is Hamiltonian operator, and ψ is the spinor wave function of photon. For the proper Lorentz group Lp, the irreducibility representations of spin s = 1 photon are D^{10}, D^{01} and $D^{1/2\ 1/2}$, respectively, and the dimension numbers of irreducibility representations corresponds to three, three and four, respectively. We choose the spinor wave function of photon as the basis vector of three-dimension irreducibility representation, i.e.

$$\psi(\vec{r},t) = \begin{pmatrix} \psi_1(\vec{r},t) \\ \psi_2(\vec{r},t) \\ \psi_3(\vec{r},t) \end{pmatrix}, \tag{47}$$

and the α~ matrices are denoted by

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \alpha_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \alpha_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (48)$$

The Eq. (47) is the spinor wave equation of photon without temperature, its plane wave solution and energy are

$$\psi(\sim r,t,) = u(p\sim)\exp[i(p\sim\cdot\sim r - Et)/\sim], \quad (49)$$

$$E = \sim\omega, \quad (50)$$

where the u(p) matrix is

$$u(p) = \begin{pmatrix} u_1(p) \\ u_2(p) \\ u_3(p) \end{pmatrix}. \quad (51)$$

The detailed theory can see the Appendix A of Ref. [15].
When the photon is in the external environment of temperature T, we should consider the thermal potential energy $Q = TS$, the Eq. (46) should be written as

$$E - TS - c\alpha\sim\cdot p\sim = 0. \quad (52)$$

By canonical quantization Eq. (53), we obtain its spinor wave equation

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t,T) = (-k_B n_i \ln n_i T^2 \frac{\partial}{\partial T} - ic\hbar\vec{\alpha}\cdot\vec{\nabla})\psi(\vec{r},t.T), \quad (53)$$

the Eq. (54) is the spinor wave equation of photon with temperature, the wave function and energy are

$$\psi(\sim r,t,T) = u(p\sim)\exp[i(p\sim\cdot\sim r - Et)/\sim]\ \varphi(T), \quad (54)$$

$$E = \sim\omega - k_B T_0 n_i \ln n_i. \quad (55)$$

Where ni is the photon numbers of photon in the $i - th$ state. If $n_i = 0,1$, the photon energy $E = \sim\omega$.

Conclusions

In this paper, we have proposed the non-Hermitian theory of quantum thermodynamics, and given the quantum thermodynamics equations, including non-relativistic and relativistic quantum theory, i.e., the temperature-dependent schrodinger equation, Dirac equation and photon equation. We give the solution of wave function and energy level with temperature, and introduced the temperature constant T0, which should be determined by the atom or molecule spectrum experiments. The theory can be applied in superconductivity, condensed state and so on, and can further study finite temperature quantum field theory.

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