Hidden gauge structure and derivation of microcanonical ensemble theory of bosons from quantum principles

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Microcanonical ensemble theory of free bosons is derived from quantum mechanics by making use of the hidden gauge structure. The relative phase interaction associated with this gauge structure, described by the Pegg-Barnett formalism, is shown to lead to perfect decoherence in the thermodynamic limit and the principle of equal *a priori* probability, simultaneously.

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I. INTRODUCTION

Quantum theoretical justification of statistical mechanics is a problem of fundamental interest [1,2]. There seem to remain several important questions yet to be answered. First of all, (i) perfect decoherence has to be realized at the level of microcanonical ensemble theory, in which there is no notion of the heat bath. (ii) The principle of equal *a priori* probability should be established in conformity with quantum principles. In addition, (iii) what is the quantum analog of classical ergodicity that may allow statistical description of a system? Consider the classical ideal gas, for example. The particles of the gas actually interact with each other in a complex manner. This interaction is responsible for validity of ergodicity but is ignored if once shifted to statistical description. Then, (iv) what is the physical property of such an interaction in quantum theory?

In this paper, we study quantum mechanical derivation of microcanonical ensemble theory of free bosons by answering to all the above questions (i)–(iv) *simultaneously*. Our discussion is based crucially on the hidden gauge structure in the system. This structure is manifested within the framework of the Pegg-Barnett unitary-phase-operator formalism. We heuristically construct the interaction Hamiltonian of a particular form, in which all relevant complex interactions needed for statistical description are assumed to be effectively summarized. Then, we show that the eigenstate of the total Hamiltonian satisfies the principle of equal *a priori* probability and, at the same time, perfect decoherence is realized in the thermodynamic limit with the help of the hidden gauge structure. Once microcanonical ensemble theory is obtained, the derivation of canonical ensemble theory is straightforward.

The unperturbed system we consider is composed of N identical bosons. The Hamiltonian reads

$$H_0=\varepsilon\sum_{i=1}^{N} a_i^\dagger a_i\,, \tag{1}$$

where $a_i^\dagger$ and a_i are the ordinary creation and annihilation operators of the ith boson satisfying the algebra, $[a_i,a_j^\dagger]=\delta_{ij}$, $[a_i,a_j]=[a_i^\dagger,a_j^\dagger]=0$, and ε is the energy of a single boson. According to the spirit of statistical mechanics, there are weak interactions between the bosons, which are responsible for the validity of statistical approach, but they can be ignored once the system is statistically described. We wish to find the interaction Hamiltonian H_1 that represents such interactions in a simple and effective way and leads to the principle of equal *a priori* probability. For this purpose, we consider the phase degree of freedom within the framework of the Pegg-Barnett formalism [3]. We shall consider only the stationary states of the isolated system, and the problem of relaxation to equilibrium will not be discussed. Also, a generalization of the present discussion to nonidentical particles is straightforward but brings extra complications.

II. PEGG-BARNETT FORMALISM

In this section, we wish to present a brief summary of the basics of the Pegg-Barnett unitary-phase-operator formalism relevant to our subsequent discussion.

The Pegg-Barnett phase state of the ith boson is given by [3]

$$|\theta_{m_i}\rangle_i=\frac{1}{\sqrt{s+1}}\sum_{n_i=0}^{s}\exp(in_i\theta_{m_i})|n_i\rangle_i\,, \tag{2}$$

$$\theta_{m_i}=\frac{2\pi m_i}{s+1}\quad(m_i=0,1,2,\ldots,s), \tag{3}$$

where $\{|n_i\rangle_i\}_{n_i=0,1,2,\ldots,s}$ is the truncated Fock basis satisfying $a_i^\dagger a_i|n_i\rangle_i=n_i|n_i\rangle_i$ and ${}_i\langle n_i|n_i'\rangle_i=\delta_{n_i,n_i'}$. $\{|\theta_{m_i}\rangle_i\}_{m_i=0,1,2,\ldots,s}$ forms an orthonormal complete system in the $(s+1)$-dimensional space. s is supposed to be large, but the limit $s\to\infty$ has to be taken after all quantum mechanical calculations.

The unitary phase operator is given by

$$\exp(i\phi_i)=\sum_{m_i=0}^{s}\exp(i\theta_{m_i})|\theta_{m_i}\rangle_i\,{}_i\langle\theta_{m_i}| =|0\rangle_i\,{}_i\langle 1|+|1\rangle_i\,{}_i\langle 2|+\cdots+|s-1\rangle_i\,{}_i\langle s|+|s\rangle_i\,{}_i\langle 0|. \tag{4}$$

Applying the operator in Eq. (4) on $|n_i\rangle_i$, we have

$$\exp(i\phi_i)|n_i\rangle_i = |n_i - 1\rangle_i \quad (n_i \neq 0),$$

$$\exp(i\phi_i)|0\rangle_i = |s\rangle_i \quad (n_i = 0). \tag{5}$$

It may be worth mentioning that the phase operator is an anomalous object and quantum-classical correspondence between the action and angle variables is violated, in general [4].

III. HIDDEN GAUGE STRUCTURE AND RELATIVE PHASE INTERACTION

It is of importance to notice that the relations in Eq. (5) remain form invariant under the following transformation:

$$|n_i\rangle_i \to |n_i, \theta_{m_i}\rangle_i = |n_i\rangle_i \exp(i\alpha_{n_i}), \tag{6}$$

$$\phi_i \to \phi_i - \partial\alpha_{n_i} \equiv \phi_i - (\alpha_{n_i+1} - \alpha_{n_i}) = \phi_i - \theta_{m_i}, \tag{7}$$

where $\alpha_{n_i} = n_i \theta_{m_i}$. This can be seen as a kind of gauge transformation, and the role of a gauge field is played by ϕ_i.

Taking into account this hidden gauge structure, we here present the following heuristically constructed interaction Hamiltonian:

$$H_1 = g\left[V^\dagger V + N \sum_{i=1}^{N} |0\rangle_{i\ i}\langle 0| \right], \tag{8}$$

$$V = \sum_{i=1}^{N} \{\exp[i(\phi_i - \theta_{m_i})] - |s\rangle_{i\ i}\langle 0|\}, \tag{9}$$

where g is a coupling constant. In Eq. (9), we have used the notational abbreviation $\Sigma_{i=1}^{N} A_i = A_1 \otimes I_2 \otimes \cdots \otimes I_N + I_1 \otimes A_2 \otimes I_3 \otimes \cdots \otimes I_N + \cdots + I_1 \otimes \cdots \otimes I_{N-1} \otimes A_N$ with I_i being the unit operator in the space of the ith boson. The subtraction term in V shows a feature of the Pegg-Barnett formalism. H_1 can be thought of as the effective Hamiltonian, in which all relevant complex interactions needed for validating statistical description are summarized. Notice that it essentially represents the relative phase interaction [5].

Since our purpose is to derive statistical mechanics of the system with H_0 and without H_1 containing anomalous objects, we here impose the condition that H_1 should vanish in the thermodynamic limit, $N \to \infty$. It turns out that this condition is fulfilled if the coupling constant is assumed to decay faster than $1/N^2$. Thus, we put

$$g = \frac{g_0}{N^{2+\delta}} \quad (\delta > 0), \tag{10}$$

where g_0 is a constant independent of N.

IV. DERIVATION OF MICROCANONICAL ENSEMBLE THEORY

Now, for a finite value of N, the normalized eigenstate of the total Hamiltonian, $H = H_0 + H_1$, is found to be

$$|M;N,[\theta_m]\rangle = \frac{1}{\sqrt{W(M,N)}} \sum_{P\{n\}} |M;[n],[\theta_m]\rangle, \tag{11}$$

with

$$|M;[n],[\theta_m]\rangle = \bigotimes_{i=1}^{N} |n_i\rangle_i \delta_{n_1+n_2+\cdots+n_N, M} \exp\left(i \sum_{i=1}^{N} n_i \theta_{m_i} \right), \tag{12}$$

$$W(M,N) = \frac{(M+N-1)!}{M!(N-1)!}, \tag{13}$$

whose energy eigenvalue is given by

$$E = M\varepsilon + \frac{g_0}{N^\delta} \quad (M = 0,1,2,...). \tag{14}$$

The symbol P stands for permutation and therefore the summation in Eq. (11) is understood to be taken over all possible combination of $\{n\} \equiv (n_1, n_2, \ldots, n_N)$. For the sake of nontriviality, the dimensionality s should be taken to be larger than M.

The space of the quantum states is enlarged by the introduction of the phase variables. The state in Eq. (11) residing in such a space is found to satisfy the following normalization condition:

$$\frac{1}{(s+1)^N} \mathrm{Tr} \sum_{m_1, m_2, \ldots, m_N = 0}^{s} |M;N,[\theta_m]\rangle\langle M;N,[\theta_m]| = 1. \tag{15}$$

Let A be a normal physical observable, which is *independent of the phase operators with anomaly*. Then, taking Eq. (15) into account, its quantum mechanical average $\langle A\rangle$ with respect to the state in Eq. (11) converges in the thermodynamic limit as well as the Pegg-Barnett limiting procedure, $s \to \infty$, as follows:

$$\langle A\rangle \to \mathrm{Tr}(A\rho_{\mathrm{mc}}), \tag{16}$$

where ρ_{mc} is given by

$$\rho_{\mathrm{mc}} = \frac{1}{W(M,N)} \sum_{P\{n\}} |n_i\rangle_{i\ i}\langle n_i| \delta_{n_1+n_2+\cdots+n_N, M}. \tag{17}$$

This is precisely the microcanonical density matrix of the bosons with the fixed energy, $E_0 = M\varepsilon$, in which perfect decoherence and the principle of equal *a priori* probability are realized simultaneously, as desired.

Finally, canonical ensemble theory can further be derived in the standard manner. The total system is divided into the objective system S and the heat bath B: $N = N_S + N_B$ ($N_S \ll N_B$), $E_0 = E_{S,M_S} + E_{B,M_B}$ with $E_{S,M_S} = M_S\varepsilon$ and $E_{B,M_B} = M_B\varepsilon$ ($M_S \ll M_B$). The total state is written as

$$|M;N,[\theta_m]\rangle = \sum_{M_S,M_B} \sqrt{\frac{W(M_S,N_S)W(M_B,N_B)}{W(M,N)}} \times |M_S;N_S,[\theta_{S,m}]\rangle_S \otimes |M_B;N_B,[\theta_{B,m}]\rangle_B \delta_{M_S+M_B,M}, \quad (18)$$

where the states of the objective system and the heat bath are, respectively, given by

$$|M_S;N_S,[\theta_{S,m}]\rangle_S = \frac{1}{\sqrt{W(M_S,N_S)}} \sum_{P\{n\}_S} |M_S;[n]_S,[\theta_{S,m}]\rangle_S, \quad (19)$$

$$|M_B;N_B,[\theta_{B,m}]\rangle_B = \frac{1}{\sqrt{W(M_B,N_B)}} \sum_{P\{n\}_S} |M_B;[n]_B,[\theta_{B,m}]\rangle_B, \quad (20)$$

in the notation analogous to Eqs. (11)–(13). The canonical density matrix of the objective system is obtained by performing the partial trace over the heat bath,

$$\rho_c = \frac{1}{(s+1)^N} \mathrm{Tr}_B \sum_{m_1,m_2,\ldots,m_N=0}^{s} |M;N,[\theta_m]\rangle\langle M;N,[\theta_m]| \cong \frac{1}{Z(\beta)} \sum_{M_S} \exp(-\beta E_{S,M_S}) \frac{1}{W(M_S,N_S)} \times \sum_{P\{n\}_S} |M_S;[n]_S\rangle_S \, {}_S\langle M_S;[n]_S|, \quad (21)$$

where

$$|M_S;[n]_S\rangle_S = \bigotimes_{i=1}^{N_S} |N_i\rangle_{S,i} \delta_{n_1+n_2+\cdots+n_{N_S},M_S}, \quad (22)$$

$$Z(\beta) = \sum_{M_S} \exp(-\beta E_{S,M_S}), \quad (23)$$

$$\beta = \frac{\partial \ln W(M_B,N_B)}{\partial E_{B,M_B}} = \frac{1}{\varepsilon} \ln\left(1+\frac{N_B}{M_B}\right) \quad (N_B \gg 1), \quad (24)$$

provided that the Boltzmann constant has been set equal to unity.

Concluding this section, we wish to emphasize the difference between the derivation of canonical ensemble theory just described above and the work of Caldeira and Leggett [6]. In Ref. [6], a system coupled with the heat bath is considered and temperature is preassigned. On the other hand, the present discussion is based on microcanonical ensemble theory for the isolated system and therefore temperature is calculated as in Eq. (24).

V. CONCLUSION

We have studied a model of free bosons with the hidden gauge structure, which may explain, in the thermodynamic limit, realization of perfect decoherence and the principle of equal *a priori* probability in microcanonical ensemble theory.

The present discussion is based crucially on the use of the phase operator. Classically, this means that the system under consideration is integrable. For a nonintegrable system, it seems essential to develop perturbation theory, in which the unperturbed integrable part may be treated by the present method or its appropriate generalizations. In this respect, one should recall that weakness of interactions is in fact a basic premise from the viewpoint of the foundations of statistical mechanics.

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[1] A. I. Khinchin, *Mathematical Foundations of Quantum Statistics* (Dover, New York, 1998).
[2] N. D. H. Dass, S. K. Rama, and B. Sathiapalan, e-print cond-mat/0112439.
[3] D. T. Pegg and S. M. Barnett, Europhys. Lett. **6**, 483 (1988); Phys. Rev. A **39**, 1665 (1989).
[4] S. Abe, Phys. Lett. A **200**, 239 (1995); **213**, 112 (1996).
[5] T. Kobayashi, Phys. Lett. A **207**, 320 (1995); **210**, 241 (1996); **222**, 26 (1996).
[6] A. O. Caldeira and A. J. Leggett, Phys. Rev. A **31**, 1059 (1985).