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Abstract. The problem of deriving statistical mechanics from the stationary Schrödinger equation is discussed. The interaction Hamiltonian, which dynamically induces entanglement of the specific type, is constructed in a unified way based on the gauge principle. It is shown how microcanonical ensembles in both Bose-Einstein and Fermi-Dirac statistics emerge in the vanishing-interaction limit.

In spite of its great success for about 1.5 centuries, classical statistical mechanics still remains challenging at the level of its fundamental principles. It is of significance to view them from the standpoint of quantum mechanics. There are a series of indications, which suggest that quantum mechanics may serve classical statistical mechanics with its foundations. The ergodic hypothesis is yet to be generically proved. The probabilistic concept in classical statistical mechanics is due to lack of knowledge about microscopic motion of a large number of particles, whereas in quantum mechanics it is a law of nature. Also, the Gibbs factor could be understood in such a way that identical particles are indistinguishable even classically, but it automatically follows from quantum mechanics. Moreover, the Planck constant is indispensable in order for the entropy to be definable in phase space. The thermal wavelength cannot be given its expression without the Planck constant. The quantum-classical correspondence in statistical mechanics is concerned not with the Planck constant but with the temperature.

Recently, a number of efforts have been made on understanding of statistical mechanics based on quantum mechanics. There, the concepts of ensemble typicality [1, 2] and eigenstate thermalization [3, 4] have been playing vital roles. In addition to these, we have recently developed a discussion [5] (see also Refs. [6, 7, 8]) about derivations of Bose-Einstein and Fermi-Dirac statistics from the stationary Schrödinger equation. In this article, we would like to summarize the discussion in a further unified way. We show how microcanonical ensembles in those statistics emerge from quantum mechanics.

In order to derive microcanonical ensemble from quantum mechanics, the following two issues are required in Ref. [5]: (I) perfect decoherence in terms of the energy eigenbasis should be realized for an isolated system, and (II) the principle of equal a priori probability has to be consistent with the solution of the stationary Schrödinger equation. The latter forces an interaction between particles to entail a specific pattern of entanglement in the quantum state.
as the solution. It should be noted that weak inter-particles interactions are in fact needed for deriving statistical mechanics even of the ideal gas: without interactions, a system could never relax to the equilibrium state. However, such interactions can be ignored when the description of the system shifts from the mechanical to the statistical mechanical.

The system we consider here consists of \( N \) identical particles with the common energy quantum \( \varepsilon \). Its free Hamiltonian has the form

\[
\hat{H}_0 = \varepsilon \sum_{i=1}^{N} \hat{n}_i. \tag{1}
\]

\( \hat{n}_i \equiv \hat{a}_i^\dagger \hat{a}_i \) is the number operator of the \( i \)th particle, where \( \hat{a}_i^\dagger \) and \( \hat{a}_i \) are the creation and annihilation operators satisfying the algebra:

\[
\left[ \hat{a}_i^\dagger, \hat{a}_j^\dagger \right]_\pm = \delta_{ij}, \quad \left[ \hat{a}_i, \hat{a}_j \right]_\pm = \left[ \hat{a}_i^\dagger, \hat{a}_j^\dagger \right]_\pm = 0 \quad \text{with the notation} \quad \left[ \hat{A}, \hat{B} \right]_\pm = \hat{A} \hat{B} \pm \hat{B} \hat{A}.
\]

The commutators (anticommutators) correspond to the bosonic (fermionic) particles. As mentioned above, it is necessary to introduce interactions between the particles. Since perfect decoherence should be realized for an isolated system as in the requirement (1), the interactions may be relevant to phases that are (approximately) conjugate to the number of the particles whose eigenstates form the energy eigenbasis. In Ref. [5], the unitary phase operator widely used in quantum optics is employed. It is defined as follows [9, 10]:

\[
\exp(i\phi_i) = \sum_{m_i=0}^s \exp(i\theta_{m_i}) |\theta_{m_i}\rangle_i \langle \theta_{m_i}|. \tag{2}
\]

Here, \( |\theta_{m_i}\rangle_i \) is the discrete phase state of the \( i \)th particle given by \( |\theta_{m_i}\rangle_i = (s+1)^{-1/2} \sum_{n_i=0}^s \exp(i\theta_{m_i}) |n_i\rangle_i \) with the normalized number state \( |n_i\rangle_i = \left( \hat{a}_i^\dagger \right)^{n_i} |0\rangle_i / \sqrt{m_i!} \) satisfying \( \hat{n}_i |n_i\rangle_i = n_i |n_i\rangle_i \) \( (n_i = 0, \ldots, s) \), where \( |0\rangle_i \) is the normalized ground state annihilated by \( \hat{a}_i \): \( \hat{a}_i |0\rangle_i = 0 \). In the bosonic case, \( s \) is a large positive integer, implying that the phase state is defined in the \( (s+1) \)-dimensional truncated space, and the limit \( s \to \infty \) has to be taken after all calculations about the phase operators and phase states [9, 10]. On the other hand, \( s \) is fixed to be \( s = 1 \) for the fermions. \( \theta_{m_i} \) is the discrete phase eigenvalue given by \( \theta_{m_i} = 2\pi m_i/(s+1) \) \( (m_i = 0, \ldots, s) \). Both \( \{|n_i\rangle_i\}_{n_i} \) and \( \{|\theta_{m_i}\rangle_i\}_{m_i} \) form the complete orthonormal systems in the \( (s+1) \)-dimensional space. Thus, \( |\theta_{m_i}\rangle_i \) is the eigenstate of the phase operator in Eq. (2): \( \exp(i\phi_i) |\theta_{m_i}\rangle_i = \exp(i\theta_{m_i}) |\theta_{m_i}\rangle_i \). As known, the phase operator cannot strictly be conjugate to the number operator since the spectrum of the number operator is discrete. The related discussions date back to Dirac [11], and one can see the phase-operator problem as a prototype of anomaly [12].

In terms of the basis \( \{|n_i\rangle_i\}_{n_i} \), the phase operator in Eq. (2) is expressed as follows:

\[
\exp(i\phi_i) = \sum_{n_i=0}^{s-1} |n_i\rangle_i \langle n_i + 1| + |s\rangle_i \langle 0|. \tag{3}
\]

What is of crucial importance for the subsequent discussion is the existence of the hidden gauge-theoretical structure. From Eq. (3), it is clear that under the \( c \)-number local (i.e., \( n_i \)-dependent) gauge transformation

\[
|n_i\rangle_i \rightarrow |n_i\rangle_i \exp(i\Lambda_{n_i, \mu_i}), \quad \Lambda_{n_i, \mu_i} = n_i \theta_{\mu_i} = \frac{2\pi \mu_i n_i}{s+1} \quad (\mu_i = 0, \ldots, s), \tag{4}
\]

\( \phi_i \) transforms as the gauge field

\[
\phi_i \rightarrow \phi_i - \partial \Lambda_{n_i, \mu_i}. \tag{5}
\]
where
\[ \partial \Lambda_{n_i, \mu_i} \equiv \Lambda_{n_{i+1}, \mu_i} - \Lambda_{n_i, \mu_i} = \theta_{\mu_i}. \]  
(6)

This structure turns out to play a central role for constructing the interaction Hamiltonian.

Let us define the following operator:
\[ \hat{v}_i = \left[ \exp(i \hat{\phi}_i) - |s_i \rangle \langle 0 | \right] \exp(-i \theta_{m_i}) q^{\hat{F}_i}, \]  
(7)
where
\[ \hat{F}_i = \sum_{j<i} \hat{n}_j \left( \hat{F}_1 \equiv 0 \right), \]  
(8)
and \( q = 1 \) \((-1)\) for the bosons (fermions). The factor \( q^{\hat{F}_i} \) is identically equal to unity for the bosons, whereas it gives rise to nontrivial sign changes for the fermions. Consider a generic number state of the fermions:
\[ |n_1, n_2, \ldots, n_N \rangle = \left( \hat{a}^\dagger_1 \right)^{n_1} \left( \hat{a}^\dagger_2 \right)^{n_2} \cdots \left( \hat{a}^\dagger_N \right)^{n_N} |0 \rangle \]  
(9)

and \( |0 \rangle = \bigotimes_{i=1}^{N} |0 \rangle_i \) (note that \( n_i! = 1 \) for the fermion). The operator in Eq. (7) can move its location on this state without changing the sign of the number state:
\[ \hat{v}_i |n_1, n_2, \ldots, n_N \rangle = \left( \hat{a}^\dagger_1 \right)^{n_1} \left( \hat{a}^\dagger_2 \right)^{n_2} \cdots \left( \hat{a}^\dagger_{i-1} \right)^{n_{i-1}} \hat{v}_i \left( \hat{a}^\dagger_i \right)^{n_i} \cdots \left( \hat{a}^\dagger_N \right)^{n_N} |0 \rangle. \]  
(10)

Now, the interaction Hamiltonian considered here reads
\[ \hat{H}_I = g \left( \hat{V}^\dagger \hat{V} + N \sum_{i=1}^{N} |0 \rangle_{i,i} \langle 0 | \right), \]  
(11)
where
\[ \hat{V} = \sum_{i=1}^{N} \hat{v}_i, \]  
(12)
and \( g \) is a coupling constant. The second term inside the brackets on the right-hand side is associated with the subtraction term in Eq. (7), which comes from the property of the phase operator in Eq. (3). Combining Eqs. (1) and (9), we obtain the total Hamiltonian
\[ \hat{H} = \hat{H}_0 + \hat{H}_I, \]  
(13)
which contains both the number and phase operators.

The stationary Schrödinger equation is given by
\[ \hat{H} |u_E \rangle = E |u_E \rangle. \]  
(14)

The solution of this equation is found to be
\[ E_{M,N} = M \varepsilon + g f(N), \]  
(15)
\[ |u_E \rangle = |M; N, [\theta_m] \rangle \]  
(16)
\[ \equiv \frac{1}{\sqrt{W(M,N)}} \sum_{P(n)} |n_1, n_2, \ldots, n_N \rangle \delta_{n_1+n_2+\cdots+n_N,M} \exp \left( i \sum_{i=1}^{N} n_i \theta_{m_i} \right). \]  
(17)

The sum in Eq. (14) implies to be taken over all independent permutations of \( (n_1, n_2, \ldots, n_N) \) with the total number of excitations being fixed to be \( M \). Accordingly, quantum entanglement of the specific type is induced by the interaction Hamiltonian. A straightforward calculation
shows that $f(N) = N^2$ for the bosons, whereas $0 < f(N) \leq N^2$ for the fermions, depending on the value of $M$ (the maximum $N^2$ is realized if $M = 1$). $W(M, N)$ is the normalization factor given by

$$W(M, N) = \frac{(M + N - 1)!}{(N - 1)! M!} \quad \text{(bosons)}, \quad \frac{N!}{(N - M)! M!} \quad \text{(fermions)},$$

which are in fact the degeneracies in Bose-Einstein and Fermi-Dirac statistics. Upon ascertaining that Eq. (14) is in fact the solution, the factor $q^F_i$ in Eq. (7) is seen to be essential for the fermions.

It is noted that by the gauge transformation in Eq. (4), the operator in Eq. (7) changes as follows: $\hat{v}_i \to \hat{v}_i \exp(i\theta_m)$. Accordingly, the interaction Hamiltonian in Eq. (9) also changes. However, since the state in Eq. (14) transforms as

$$|M; N, [\theta_m]\rangle \to |M; N, [\theta_m + \theta_m]\rangle,$$

Eq. (12) holds for the gauge transformed Hamiltonian and eigenstate with the invariant energy eigenvalues.

Now, Eq. (16) means that the phases in the eigenstate is indeterminate. In the vanishing-interaction limit

$$g \to 0,$$

which has been mentioned earlier, the phase operators disappear from the theory. This leads to a situation somewhat analogous to random phases, and therefore the phases are eliminated from the density matrix

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

$$= \frac{1}{W(M, N)} \sum_{P[n]} |n_1, n_2, \ldots, n_N\rangle \langle n_1, n_2, \ldots, n_N| \delta_{n_1 + n_2 + \ldots + n_N, M}.$$  

This is precisely the density matrix in microcanonical ensemble theory, and perfect decoherence in the energy eigenbasis and the equal probability are simultaneously realized, as desired.

Canonical ensemble can be obtained from microcanonical ensemble in a straightforward way. The total isolated system is divided into the objective subsystem and the environmental system, provided that the latter should be much larger than the former. Then, the partial trace is taken over the environmental system to obtain the canonical density matrix (for details, see Ref. [5]).

Thus, we have seen how Bose-Einstein and Fermi-Dirac statistics can be derived from quantum mechanics. From them, classical statistical mechanics simply appears from these in the high-temperature regime, as widely known.

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