論文の内容の要旨

論文題目

Theoretical Study on the Foundation of Statistical Mechanics in Isolated Quantum Systems

(孤立量子系における統計力学の基礎に関する理論的研究)

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The main theme of this thesis is the foundation of statistical mechanics in isolated quantum systems: how equilibrium states, or macroscopically unchanging states, emerge in the course of the unitary time evolution, why they are well described by the microcanonical ensemble, and how the thermodynamic entropy is interpreted from a quantum-mechanical viewpoint.

Isolated quantum systems are by definition not in contact with a heat bath and, thus, they never lose their memory of the initial state to reach thermal equilibrium by throwing away the information to the bath. Therefore, to address the questions raised above, we must find out the inherent ability of isolated quantum systems to undergo thermalization.

The foundation has been studied since the early 20th century because an isolated system plays the most fundamental role in statistical mechanics. Presupposing that the microcanonical ensemble describes thermal equilibrium states in isolated systems, the canonical ensemble, for example, is deduced in systems in contact with a heat bath. Despite its importance, the foundation is still only presupposed and has not been fully proven yet.

Recently, the theme has attracted renewed attention because isolated quantum systems have experimentally been realized using ultracold atoms, which are trapped by lasers in a high vacuum. Until then, it had been of purely theoretical interest, and thermalization of most quantum systems in reality had often been ascribed to the coupling with their environment. Now that thermalization is actually observed in ultracold atom experiments, the theme is of interest not only theoretically but also experimentally.

One of the difficulties in deriving equilibration, or the approach to a macroscopically unchanging state, within the unitary time evolution is the fact that the evolution has no fixed point. An initial pure state $|\psi\rangle$ evolves so that the state at time t is given by $|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}t} |\psi\rangle$, where $\hat{H}$ is a time-independent Hamiltonian and the Planck constant is set to unity. According to this formula, the initial state never converges to any point and keeps changing forever. Seemingly, there cannot be equilibration in the course of the unitary time evolution.

The key to resolving this enigma lies in the fact that equilibration implies no state change only macroscopically. The state vector $|\psi(t)\rangle$ at time t contains the complete information about all physical observables including microscopic ones. Let us consider, for example, a model of spin-1/2's on a lattice of N sites that has no symmetry. The pure state $|\psi(t)\rangle$ is a 2^N-dimensional vector, which gives expectation values for all the independent Hermitian operators including the local magnetizations and the two-point spin correlations that are experimentally measurable. However, the Hermitian operators also involve the full N-point spin correlations that are de facto unmeasurable in a large system, and the number of them amounts to 3^N (x-, y-, and z-directions of the spin component at each site). These unmeasurable observables are the overwhelming majority compared with the few-spin correlations since the number of them are of a polynomial order of N. Thus, even if $|\psi(t)\rangle$'s are all different at each t, most of them can share the expectation values of a few-spin correlations, which is essentially an equilibrium state appearing under the unitary time evolution.

The striking fact that almost all pure states look the same as far as only macroscopically measurable observables are concerned is called the "typicality" and has been noticed since the late 20th century. A new approach to the foundation of quantum statistical mechanics based on the typicality has been widely studied since then as an alternative to the ergodicity approach. This thesis archives the previous and original studies on the new approach.

Previous studies have revealed that equilibration described above is interpreted as dephasing between (many-body) energy eigenstates. If we denote by $\{|E_n\rangle\}_n$ the eigenstates of $\hat{H}$ with eigenenergies $\{E_n\}_n$, the time evolution is represented as $|\psi(t)\rangle = \sum_n c_n \mathrm{e}^{-\mathrm{i}E_n t} |E_n\rangle$, where $c_n \equiv \langle E_n|\psi\rangle$ is the expansion coefficients of the initial state in the energy eigenbasis. Assuming that the spectrum is not degenerate, the infinite-time average of the density matrix is given by $\overline{|\psi(t)\rangle \langle\psi(t)|} = \sum_{m,n} c_n^* c_m \overline{\mathrm{e}^{\mathrm{i}(E_n - E_m)t}} |E_m\rangle \langle E_n| = \sum_n |c_n|^2 \langle E_n| |E_n\rangle \equiv \hat{\rho}_{\mathrm{DE}}$, where $\overline{\cdots}$ denotes the infinite-time average and $\hat{\rho}_{\mathrm{DE}}$ is called the diagonal ensemble. Here, the off-diagonal, or $m \neq n$, contributions vanish due to dephasing.

The equilibrium state characterized by the diagonal ensemble still retains the memory of the initial state, or $|c_n|^2$'s and looks different from the microcanonical ensemble $\hat{\rho}_{\mathrm{mic}}(E) =$

$W(E,\delta_{\text{mic}})^{-1}\sum_{n \text{ s.t. } |E_n-E|\leq\delta_{\text{mic}}} |E_n\rangle\langle E_n|$, where $E = \langle\psi|\hat{H}|\psi\rangle$ is the energy of the system, δ_{mic} is a macroscopically small energy, and $W(E,\delta_{\text{mic}})$ denotes the number of energy eigenstates in the energy window $[E-\delta_{\text{mic}}, E+\delta_{\text{mic}}]$. Whereas each eigenstate has, in $\hat{\rho}_{\text{DE}}$, weight $|c_n|^2$ determined by the initial state, it does, in $\hat{\rho}_{\text{mic}}(E)$, the equal weight in the energy window.

The eigenstate thermalization hypothesis (ETH) has been proposed to ensure that the diagonal and microcanonical ensembles are equivalent in the thermodynamic limit when only macroscopically measurable observables are concerned. Namely, in the above example of the spin-1/2 model, the eigenstate expectation value $\langle E_n|\hat{O}|E_n\rangle$ of a few-site observable $\hat{O}$ becomes independent of n within a small energy window in the thermodynamic limit. More and more pieces of evidence of the ETH have been accumulated in recent years.

Although the ETH gives an answer to the question of why the microcanonical ensemble describes well equilibrium states resulting from the unitary evolution in the thermodynamic limit, it has not been addressed how accurately it does in small isolated quantum systems. This question is of fundamental interest related to how thermodynamics emerges as the system size increases. Besides, it would gain importance now that ultracold atomic systems with a few fermions have been experimentally realized at high fidelity.

The first original study archived in this thesis, on which I have made the principal contribution, is on the accuracy of the microcanonical ensemble in small isolated quantum systems. We have considered a one-dimensional nonintegrable hard-core Bose-Hubbard model at the 1/3 filling with the nearest- and next-nearest-neighbor hopping and interaction, where the number of sites L ranges from 15 to 24. By using the full numerical diagonalization of the Hamiltonian, we have conducted the numerical experiments of the quantum quench of the nearest-neighbor interaction and analyzed the equilibrium states reached after the quench. For each initial state, which is an energy eigenstate around the middle of the spectrum, we have calculated the difference between the diagonal and microcanonical ensemble averages, $\text{tr}(\hat{\rho}_{\text{DE}}\hat{O})$ and $\text{tr}(\hat{\rho}_{\text{mic}}(E)\hat{O})$, of a few-body observable $\hat{O}$ chosen to be the correlations in the boson numbers at the nearest- or next-nearest neighbors. We find that the distribution of the difference $\text{tr}(\hat{\rho}_{\text{DE}}\hat{O})-\text{tr}(\hat{\rho}_{\text{mic}}(E)\hat{O})$ obtained for each initial state peaks at zero with the width becoming narrower as L increases. Then, focusing on the width of the distribution, we have shown that the root mean square of the differences vanishes proportionally to D^{-1}, where D denotes the dimension of the Hilbert space. This implies a surprisingly rapid convergence of the difference to zero because D grows exponentially as L increases.

The D^{-1} scaling of the accuracy of the microcanonical ensemble is much faster than the ETH prediction of the $D^{-1/2}$ scaling in a finite-size system, and implies that the microcanonical ensemble is quite accurate in a system already with several particles. In fact, in our model with only 8 bosons on $L = 24$ sites, the relative error is already as small as 0.01%, which will improve approximately by one order of magnitude every time we increase the number of bosons by one.

We have identified the physical origin of the discrepancy between the D^{-1} and $D^{-1/2}$ scalings with the fact that there are no correlation between $|c_n|^2$'s, or the weights on each many-body energy eigenstates. This is because, if so, the difference between the diagonal and microcanonical ensemble averages are suppressed by the extra factor of $D_{\mathrm{eff}}^{-1/2}$ due to the law of large numbers, where D_{eff} denotes the effective number of energy eigenstates involved in $|\psi\rangle$, which is proportional to D in our quench problem.

The other original result of the present thesis is on the thermodynamic entropy of the equilibrium state reached in the course of the unitary time evolution. The von Neumann entropy has been used as the microscopic definition of the thermodynamic entropy because it is consistent with thermodynamics when applied to the statistical ensembles such as the canonical ensembles. However, in an isolated quantum system, the von Neumann entropy is inconsistent with the second law of thermodynamics since it never changes upon an arbitrary unitary external operation whether or not it is quasi-static. Thus, the von Neumann entropy needs to be replaced by an appropriate entropy that gives the thermodynamic entropy of equilibrium states in isolated quantum systems.

We propose the diagonal entropy, which is the Shannon entropy in the energy eigenbasis, as the right candidate for the microscopic definition by showing that it is consistent with the second law of thermodynamics in the following sense. We assume that an initial state evolves according to a Hamiltonian $\hat{H}_0$, where equilibration occurs, and apply an external operation denoted by an arbitrary unitary operator $\hat{V}$ at time $t = \tau$. We regard the diagonal entropy after the operation $S'(\tau)$ as a function of τ and compare it with that before the operation, S_0. We have shown that, in a large system, the infinite-time average of $S'(\tau)$ in terms of τ is greater than (or equal to) S_0, and that the fluctuation of $S'(\tau)$ around the infinite-time average vanishes. These results imply that the diagonal entropy increases (or stays constant) for almost all operation timings.

We note that an asymmetry between the increase and decrease of the diagonal entropy emerges notwithstanding the time-reversal symmetry of the unitary time evolution. We argue that the asymmetry derives from the fact that the physically allowed states in the unitary time evolution with a time-independent Hamiltonian are restricted to a subspace rather than the entire Hilbert space.