Classical equipartition theorem and its universal quantum counterpart

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In classical statistical physics, the theorem on equipartition of kinetic energy is one of the most universal relation. It states that for a system in thermodynamic equilibrium of temperature T, the mean kinetic energy E per one degree of freedom is equal to E = k T/2, where k is the Boltzmann constant. E does not depend on a number of particles in the system, the form of the potential force which acts on them, the form of interaction between particles and strength of coupling between the system and thermostat. It depends only on the thermostat temperature T. On the contrary, for quantum systems, the mean kinetic energy is not equally shared among all degrees of freedom and the theorem fails. The question arises whether one can formulate a similar and universal relation for the mean kinetic energy of quantum systems at the thermodynamic equilibrium state. The answer is: Yes, if the composed quantum system (Thermostat + System) is at the Gibbs canonical state of arbitrary temperature [1]. The relation holds true for all quantum systems composed of an arbitrary strength (valid both in weak and strong coupling regimes).

For a system of one degree of freedom this quantum counterpart, which can be called the energy partition theorem, has the appealing form:

(1)
$$E = \int e(\omega) P(\omega) d\omega,$$

where $e(\omega)$ has exactly the same form as the average kinetic energy of the quantum harmonic oscillator with the frequency ω weakly coupled to thermostat of temperature T and $P(\omega)$ is a probability density on a positive half-line of real numbers. The explicit form of the probability density $P(\omega)$ depends on the microscopic model of the Thermostat + System and has been derived for several exactly solved quantum systems like as a free particle or quantum oscillator [2-7]. The relation (1) is a generalization of the classical energy equipartition theorem for quantum systems and in the high temperature limit it reduces to its classical form E = kT/2. In the low temperature regime [5] it exhibits interesting properties which will be discussed in the lecture.

References

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