Quantum statistical mechanical design of nanomachines

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Nanomachines have been attracting much attention, and have been studied and developed both experimentally and theoretically in recent years. In particular, experimental studies of molecular machines have made remarkable progress, which, however, have been designed empirically or intuitively. Thus theoretical studies that are capable of providing some insights for those experiments are required.
We here propose a quantum statistical-mechanical method of designing nanomachimes that fully takes quantum effects and entropy effects into consideration. The method enable one to calculate properties and performances of nanomachines, including the response times when they are controlled by physical stimulations such as an external magnetic field. Furthermore, one can applies the method to any minute quantum system, so that the method will open a way to designing nanomachines made of almost minimum degrees of freedom.
We couple mainly two theoretical techniques for the method: One is the thermal pure quantum (TPQ) formulation of statistical mechanics [1, 2], which we here generalize to systems without translational invariacne to analyze nanomachines. The other is the Chebyshev polynomial expansion method [3], which we here apply to nanomachines with the help of the TPQ formulation.
As the first nanomachine that is obtained by our method, we present a novel minute machine whose shape is changed by application of a pulsed external field, like a catalyst whose catalytic property is changed by redox. The system shows a characteristic shape before application of an external field, and by application of a pulsed external field the system exhibits a uniform shape. Further application of an external field makes the system to show another characteristic shape. This shape can be erased by even further application of an external field. By utilizing both quantum effects and entropy effects, we realize this system on a lattice without fine tuning of parameters on individual lattice points and with the number of principal parameters less than the number of shapes the system shows.

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