A Quantum Carnot Engine in Three-Dimensions

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Abstract

A simple quantum engine is designed which makes use of the closed-form solution for the energy eigenvalues of the Schrödinger equation under an infinite three-dimensional spherical potential well. A reversible cycle is defined for this system and made to operate in such a way that equations of state can be formulated for it on each leg of its cycle. For a closed, reversible cycle, a quantum Clausius equation can be obtained.

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1 Introduction.

A classical heat engine takes energy from a high-temperature heat reservoir such that some of this energy is converted into mechanical work. In general, some of the energy taken from the heat reservoir is not converted into mechanical energy, but ends up in a low-temperature reservoir. This is to say that a heat engine is not perfectly efficient. Maximum efficiency is achieved by a classical engine which operates between a high-temperature and low-temperature
reservoir provided it is reversible. While it is not possible to construct a working heat engine that is perfectly reversible, a mathematical model of an ideal heat engine that is not only reversible but also cyclic was proposed by Carnot. The standard Carnot engine consists of a cylinder which contains an ideal gas that is alternately placed in thermal contact with high-temperature and low-temperature heat reservoirs whose temperatures are $T_H$ and $T_C$, respectively. If we have two such sources, we can transform heat into work by a process called a Carnot cycle [1].

It is worth asking whether a quantum version of the Carnot engine can be created or even imagined [2-3]. Although each cycle of a classical Carnot engine is infinitely long, it has been thought that by choosing a specific form of time-dependent Hamiltonian, it would be possible to construct a quantum mechanical cycle over a short time scale. Instead of a classical system of a gas, a quantum mechanical system which is composed of a single particle in contact with a reservoir will be introduced here. The model which will constitute the system will consist of a three-dimensional spherical potential well. It has long been known that the energy eigenvalues for this model can be obtained in closed form [4]. The statistical ensemble of many such identically prepared systems would be characterized by a density matrix. The system can be allowed to interact weakly with its environment. The intention of considering this type of system is to try to improve the understanding of the relationship between the different areas of thermodynamics and quantum mechanics. A model similar to this one has been considered [5], but it was entirely one-dimensional but did consist of a system with an infinite set of levels as does the one here. Other types of quantum mechanical engine have been considered [6], but the cycle imagined here has the advantage of simplicity without the worry about such matters as complicated state preparations. The Szilard engine [7-8] is another model which involves both quantum mechanics and statistical thermodynamics, and has the same basic goal underneath, but it involves several classical features as well. Since observations must be performed by an observer, this would be expected to a certain degree [9]. It will be seen that these results lead naturally to a quantum analogue of the Clausius equality for a reversible cycle. The model proposed here will try to eliminate some of these drawbacks and consider a fundamentally quantum mechanical process.
2 The Physical Model

A quantum mechanical engine will be constructed here by making use of a spherically symmetric infinite-state square well in three-dimensional space. It is hoped that this might provide motivation to consider real experimental realizations which might be envisioned in the future. Such an engine may be feasible and be made to yield observations. The equations of state can be derived for isoenergetic and adiabatic processes based on the fact that this model can be solved in closed form for the energies. This model will be a three-dimensional version of the one-dimensional box of length $a$, but will have spherical symmetry. The central potential is given by a potential energy function described by

$$U(r) = \begin{cases} 0, & r < a, \\ \infty, & r > a. \end{cases} \quad (2.1)$$

This potential represents a spherical region in three-dimensional space which has impenetrable walls. The particle is prevented from escaping from the region and the motion is restricted to the spherical region $r < a$ in three space. The radial time independent Schrödinger equation which applies inside the well $r < a$ is given by

$$R''(r) + \frac{2}{r} R'(r) - \frac{l(l+1)}{r^2} R(r) + k^2 R(r) = 0, \quad (2.2)$$

where $k$ is given by

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \quad (2.3)$$

It is useful to rescale the length in (2.2) by introducing $\rho = kr$, so it becomes

$$\ddot{R}(\rho) + \frac{2}{\rho} \dot{R}(\rho) + \left[1 + \frac{l(l+1)}{\rho^2}\right] R(\rho) = 0. \quad (2.4)$$

This is a spherical Bessel equation whose solutions are given by spherical Bessel functions $j_l(\rho)$ and spherical Neumann functions $n_l(\rho)$. Since the origin is included in the spherical region so the spherical Neumann functions are excluded from the solution since they are not defined at $r = 0$. The solution $\varphi_{n,l}(r)$ in the region $r < a$ is given by

$$R_{l}^{(1)}(r) = C j_l(kr), \quad R_{l}^{(2)}(r) = 0, \quad r < a. \quad (2.5)$$
The bound state energies are defined by the condition that $\varphi_{n,l}(r)$ must vanish at both the origin and at the surface of the sphere at $r = a$, that is to say $j_l(ka) = 0$. The quantum number $n$ will designate the order of the zero. Since $j_l(kr)$ oscillates indefinitely, there are an infinite number of such zeros. There are consequently an infinite number of energy levels which fit into this spherical well for each value of the orbital angular momentum quantum number. The energy eigenvalues are characterized by the two quantum numbers $n$ and $l$. They are related to $k_{n,l}$ by the fact that $k_{n,l}a$ must be a root of $j_l(kr)$,

$$k_{n,l}a = \xi_{n,l}.$$  

In (2.6), $\xi_{n,l}$ is the $n$-th root of the $l$-th spherical Bessel function. Substituting into $k$ in (2.3), the equation can be solved for the energies to yield,

$$E_{n,l} = \left(\frac{\hbar^2}{2ma^2}\right)\xi_{n,l}^2.$$  

(2.7)

The lowest energy corresponds to $n = 1$, the second to $n = 2$ and so forth. It can be seen from (2.7) that the energies depend inversely on the square of the well radius. To obtain equations of state, we would want to express the energies in terms of the volume $V$ of the well. Since the region has been defined to be spherical, it is known exactly how the radius variable is related to the volume. Substituting $a = (3V/4\pi)^{1/3}$ into (2.7), the energy can be written in the form,

$$E_{n,l} = \left(\frac{4\pi}{3}\right)^{2/3} \frac{\hbar^2}{2mV^{2/3}}\xi_{n,l}^2.$$  

(2.8)

Assume the radius of the well is initially $r = a_1$ which corresponds to the volume $V_1$ and that the initial energy of the system is a fixed constant $E_H$. The initial state $\psi(x)$ of the system is a linear combination of the energy eigenstates given as $\psi(x) = \sum_{n=1}^{\infty} b_n\varphi_{n,l}(r)$. It will suffice to consider the system for a single value of the angular momentum quantum number, thus

$$\sum_{n=1}^{\infty} p_nE_{n,l}(V_1) = E_H.$$  

(2.9)

In (2.9), $p_n = |b_n|^2$ and $E_H$ is bounded below by $E_H \geq E_1(V_1)$. The pure state $\psi(x)$ characterizes a typical element of the ensemble whose statistical properties are determined by the density matrix given in terms of energy eigenstates by $\rho_{mn} = p_n\delta_{mn}$. This serves to establish the basic physics of the model.
3 A Quantum Cycle for the System

The objective here is to define a quantum process on the particle in the well starting from this initial configuration. The quantum cycle is defined as follows: first, the well expands isoenergetically. This means the width of the well increases infinitely slowly while the system is kept in contact with an energy bath. If the system were isolated during such an expansion, the system should remain in its initial state by the quantum adiabatic theorem. Thus the $|b_n|$ would remain constant, and the energy of the system, or expectation value of the Hamiltonian, would vary in volume as $V^{-2/3}$ if the system were isolated. Throughout the expansion, energy is simultaneously pumped into the system to compensate for the decrease in energy. This expectation value of the Hamiltonian remains constant due to excitation of higher energy levels, thus increasing the values of the $p_n$ terms in (2.9).

During the isoenergetic expansion, work is done by the radial pressure $P$ on the outer spherical wall of the well. There is a contribution to this force due to the $n$-th energy eigenstate of

$$f_n = \tau \frac{\hbar^2}{3mV^{5/3}} \xi^2_{n,l}, \quad \tau = (\frac{4\pi}{3})^{2/3}.$$

The force $P$ is given by the expectation value $P = \sum_n p_n f_n$, and so using (2.9), the equation of state during an isoenergetic process is obtained,

$$PV = \frac{2}{3} E_H.$$

The expansion coefficients $b_n$ of the wavefunction change as a function of volume as the well goes from $V_1$ to $V_2$.

During the second phase of the cycle, there occurs an adiabatic expansion of the system. In the course of such an expansion, the eigenstates change as a function of $V$, however, the $|b_n|$ remain constant. This means the expectation value of the Hamiltonian $E = \sum_n p_n E_n$ decreases during the process because each $E_n$ decreases with increasing $V$ while the $p_n$ remain fixed. The force $P$ is determined by differentiating the energy $E$ with respect to $V$,

$$PV^{5/3} = \frac{2}{3} V_2^{2/3} E_H.$$

This is a quantum analogue of the corresponding equation of state for a classical gas. The system expands adiabatically until its volume reaches $V = V_3$, and at this point, the expectation value of the Hamiltonian decreases to $E_C$. 
The squared coefficients $p_n$ of the wave function remain constant during an adiabatic process. The value of $E_C$ is given by

$$E_C = \frac{V_2^{2/3}}{V_3^{2/3}} E_H.$$  \hfill (3.4)

Following the expansion, the system is compressed isoenergetically until $V = V_4$ with the expectation value of the Hamiltonian fixed at $E_C$, and finally, it is compressed adiabatically until the radius of the region returns to its initial value. The cycle is reversible and the efficiency of the quantum engine is given by

$$\eta = 1 - \frac{E_C}{E_H}.$$  \hfill (3.5)

This expression is analogous to the classical thermodynamic result of Carnot.

A quantum system has been displayed with a slowly changing time-dependent Hamiltonian from which work can be extracted. To design this system, it was important to be able to introduce the concept of an energy bath that maintains the expectation value of the Hamiltonian. During an isoenergetic expansion, the amount of energy transferred to the system which maintains the expectation value of the Hamiltonian is determined by (3.2) by means of

$$Q_H = \int_{V_1}^{V_2} dV P(V) = \frac{2}{3} E_H \ln \left( \frac{V_2}{V_1} \right).$$  \hfill (3.6)

The amount of energy absorbed during an isoenergetic compression can be determined in a similar manner with the result that $Q_C = -\left(\frac{2}{3}\right) E_C \ln(V_3/V_4)$. Thus, for a closed, reversible cycle, we obtain a quantum version of the Clausius equality,

$$\frac{Q_H}{E_H} + \frac{Q_C}{E_C} = 0.$$  \hfill (3.7)

This follows since for a closed cycle, $V_2/V_1 = V_3/V_4$.

4 References

[2] H. S. Leff and A. F. Rex (eds), Maxwell’s Demon, Entropy, Information,

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