

Comment on 'Quantum-mechanical Carnot engine'

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COMMENT

Comment on ‘Quantum-mechanical Carnot engine’**K Bhattacharyya¹ and S Mukhopadhyay**

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Abstract

The equations governing adiabatic and isothermal quantum processes involved in an ideal two-state quantum heat engine are modified when the ideality restriction is removed. We seek and study a few situations to determine the nature and magnitude of the modifications. If one confines such systems well within the classical turning point, we show how one can profitably employ the Wilson–Sommerfeld quantization rule to estimate the leading correction terms due to non-ideality. The endeavour is likely to be important in studies on practical quantum engines.

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In a recent work [1], Bender *et al* constructed an elegant quantum-mechanical equivalent of the Carnot engine. It involves primarily two energy states and two key processes, one isothermal and one adiabatic, for which appropriate definitions pertaining to the quantum domain have been put forward. The quantum adiabatic process is governed by the property of a *particular* eigenvalue, while the isothermal one is characterized by the eigenvalue *spectra*. The working substance in a classical Carnot cycle is an ideal gas. In dealing with the quantum case, this has been replaced by the particle-in-a-box (PB) model. As a result, the classical equation governing an adiabatic process for a one-dimensional ideal gas,

$$PV^3 = C_A \quad (1)$$

where C_A denotes some constant, is replaced by

$$F(L)L^3 = C_A(q) \quad (2)$$

in the quantum description. Here the particle is confined in $(0, L)$ in one dimension, $F(L) = -dE(L)/dL$ defines the force and $C_A(q)$ is another constant. Similarly, for the same systems, the respective equations describing an isothermal process are

$$PV = C_I \quad (3)$$

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and

$$F(L)L = C_I(q). \quad (4)$$

Now, the point is that the Carnot engine is not a *real* engine; one cannot work with an ideal gas in practical situations. Likewise, the PB system is an idealization at the quantum level. Thus, it is difficult for the PB to model a wide variety of practical quantum heat engines. One way to take account of some kind of non-ideality in the quantum domain is to consider a varying potential field in $(0, L)$. However, there is no natural system that straightforwardly fits into the situation barring the case of the supersymmetric (SUSY) partner potential of the PB [2]. This implies that results (2) and (4) are restrictive. Therefore, we search for a class of *non-ideal* quantum systems and examine (a) how far relations (2) and (4) remain valid and (b) under what situations we can predict the major corrections to (2) and (4). The analysis will help us to understand quantum adiabatic and isothermal processes, as introduced in [1], in a better way. One can also extend the original work to study *real* quantum heat engines via this route.

We choose a general one-dimensional Hamiltonian

$$H = -\mathrm{d}^2/\mathrm{d}x^2 + v(x) \quad (5)$$

to describe the system. The system, however, is *confined* in $(0, L)$. This means that we have to deal with a *compressed* system (see, e.g., [3] and references therein). These systems are useful in a variety of practical cases. We shall see the importance here too, in modifying results (2) and (4), characteristic of quantum adiabatic and isothermal processes, of arbitrary one-dimensional Hamiltonians. One advantage is immediate in the present context. Like the PB case, the length L can here be varied to interpret the force $F(L)$. However, introduction of artificial boundaries makes these systems analytically intractable. Therefore, we solve the eigenvalue problem numerically corresponding to (5) by following a linear variational strategy [4] for two sample cases: $v(x) = x^2$ and $v(x) = x^4$. To this end, the Hamiltonian matrix is constructed by employing the PB bases in $(0, L)$ and is then diagonalized at various L -values of interest to obtain the relevant quantities.

First, we consider the adiabatic case. Table 1 shows a few results over a range of L -values. Note that $C_A(q)$ is dependent on the quantum number (n) and is thus a property of an energy eigenstate. Here we choose, as [1] did, the ground ($n = 1$) and first excited ($n = 2$) states. We happily find from the data that for large compression ($L < 1$), both the systems obey (2) reasonably, if we allow a tolerance of around 3%. They also approach the exact PB predictions for $C_A(q)$ for states $n = 1$ and 2 as L decreases. Nevertheless, the error grows very rapidly with L beyond $L = 1$, the more so for the lower state.

A sufficiently compressed quantum system defined by (5) will have little to contribute beyond the classical turning point. Therefore, semiclassical and quantum predictions, which usually differ mainly due to the quantum contribution beyond the turning point, are expected to agree reasonably when L is considerably less than the turning point corresponding to the uncompressed problem. As a result, it should be possible to explain semi-quantitatively the above departure from ideality via the semiclassical Wilson–Sommerfeld (WS) quantization rule [5]. Putting accordingly

$$\int_0^L (E - v(x))^{1/2} \mathrm{d}x = n\pi/2 \quad (6)$$

with $h = 2\pi$ and $m = \frac{1}{2}$ (see equation (5)), we obtain the following result for any power-law potential of the type $v(x) = x^{2N}$:

$$E = (n\pi/L)^2 + \frac{1}{2n+1}L^{2N} + \mathrm{O}(L^{4N+2}/n^2\pi^2) \quad L^{N+1} \ll n\pi \quad (7)$$

Table 1. Departures of $F(L)L^3$ from constancy and ideality for quantum adiabatic processes involving x^{2N} -type potentials in $(0, L)$ ($C_A(q) = 2(n\pi)^2$).

$v(x)$	L	State			
		$n = 1$		$n = 2$	
		$F(L)$	$F(L)L^3$	$F(L)$	$F(L)L^3$
x^2	2.0	1.536	12.286	8.542	68.335
	1.5	5.050	17.045	22.419	75.666
	1.0	19.181	19.181	78.314	78.314
	0.75	46.367	19.561	186.675	78.754
	0.5	157.631	19.704	631.334	78.917
	0.25	1 263.17	19.737	5 053.08	78.954
	0.1	19 739.1	19.739	78 956.8	78.957
x^4	2.0	0.574	4.589	4.923	39.380
	1.5	4.493	15.163	21.038	71.003
	1.0	19.288	19.288	78.254	78.254
	0.75	46.597	19.658	186.860	78.832
	0.5	157.857	19.732	631.567	78.946
	0.25	1 263.30	19.739	5 053.23	78.957
	0.1	19 739.2	19.739	78 956.8	78.957

and hence

$$F(L)L^3 = C_A(q) - \frac{2N}{2N + 1}L^{2(N+1)} + \dots \tag{8}$$

after some manipulations. Here $C_A(q)$ is the PB estimate of $2(n\pi)^2$. We find now that $C_A(q)$ decreases from its limiting, constant value. Furthermore, equation (8) shows very clearly the N dependence of the primary correction term. It also reveals that this leading term is independent of the quantum number. Employing (8), one can compare the WS predictions for $F(L)L^3$ against exact results displayed in table 1. The trend is correct; the agreement is also remarkable, keeping in mind the restriction $L^{N+1} \ll n\pi$. Within $L = 1$, we checked that the maximum error is less than 0.6%. Choosing a more general $v(x)$ in (5), of the form

$$v(x) = \sum_j a_j x^j \tag{9}$$

we find in an analogous manner that

$$F(L)L^3 = C_A(q) - a_1 L^3/2 + \dots \tag{10}$$

Once again, the leading correction term to ideality is n -independent. The sign, however, depends on the nature of $v(x)$. One thus achieves the desired first-order modification to (2) in this general situation.

Next, we consider the isothermal case. Here, we prefer to remain roughly within $L = 1$ so that the WS predictions retain some validity. Accordingly, we start from the ground state at $L = L_1 = 0.5$ and study an expansion process. Table 2 displays relevant results for x^2 and x^4 potentials, as before, by following the recommended strategy [1]. As L increases, probability of the ground state $|a_1|^2$ decreases to finally become zero; but, $F(L)L$ too is seen to gradually reduce. It maintains constancy within 1.5% in the chosen interval. To analyse the behaviour, we again employ (7). Conservation of average energy leads to

$$|a_1|^2 = \frac{4}{3} - \frac{1}{3}(L/L_1)^2 + \frac{L^2}{3\pi^2(2N + 1)}(L^{2N} - L_1^{2N}) + \dots \tag{11}$$

Table 2. Effect of non-ideality in quantum isothermal expansion processes from the $n = 1$ state involving x^{2N} -type potentials in $(0, L)$ ($C_I(q) = 8\pi^2$ in both cases).

$v(x)$	L	$ a_1 ^2$	$F(L)L$
x^2	0.5	1.0	78.816
	0.6	0.8537	78.683
	0.7	0.6812	78.521
	0.8	0.4827	78.325
	0.9	0.2583	78.091
	1.0	0.0084	77.814
x^4	0.5	1.0	78.928
	0.6	0.8534	78.875
	0.7	0.6804	78.779
	0.8	0.4811	78.613
	0.9	0.2560	78.342
	1.0	0.0057	77.920

yielding finally

$$F(L)L = C_I(q) + \frac{2}{2N+1}L_1^{2N} - \frac{2N+2}{2N+1}L^{2N} + \dots \quad (12)$$

with $C_I(q) = 2(\pi/L_1)^2$. One can now see the effectiveness of the WS predictions. From (11), we first note that here L_2 , the maximum length up to which the isothermal expansion can continue, is *greater* than $2L_1$. At $L = 2L_1 = 1.0$, we obtain $|a_1|^2$ from (11) to be 0.008 44 for $v(x) = x^2$ and 0.006 33 for $v(x) = x^4$. The accurate values shown in table 2 are quite close. Secondly, displayed results for $F(L)L$ also agree with calculations based on (12) to within 0.2%. Finally, we note that (12) contains two extra terms compared with (4). Of these, the first correction term modifies the *constant*, while the second one accounts for change with L . In a general case, with $v(x)$ given by form (9), one will find

$$F(L)L = C_I(q) + a_1L_1 - 3a_1L/2 + \dots \quad (13)$$

in place of (12). The basic feature, however, remains the same. One extra term modifies the constant; the other is a function of L . Thus, we obtain leading corrections to (4).

In summary, Bender *et al* [1], on their way to construct a quantum Carnot cycle, put forward novel definitions of quantum adiabatic and isothermal processes. They worked out characteristic features (namely equations (2) and (4)) of these processes too that are central to establish the analogy sought. However, these features are ‘ideal’. Possibly two systems, the PB and its SUSY partner, obey such features. Here we show that their definitions apply to compressed systems as well. Thus, one can now study the above processes in a wide variety of situations. We also outline how and when one would find partially modified equations describing these processes when the potential in $(0, L)$ has some spatial dependence. We achieve this via the WS quantization rule. In studying analogies between real heat engines and their quantum counterparts, work along similar lines may be useful.

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