Quantum Force due to Distinct Boundary Conditions

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Abstract. We calculate the quantum statistical force acting on a partition wall that divides a one dimensional box into two halves. The two half boxes contain the same (fixed) number of noninteracting bosons, are kept at the same temperature, and admit the same boundary conditions at the outer walls; the only difference is the distinct boundary conditions imposed at the two sides of the partition wall. The net force acting on the partition wall is nonzero at zero temperature and remains almost constant for low temperatures. As the temperature increases, the force starts to decrease considerably, but after reaching a minimum it starts to increase, and tends to infinity with a square-root-of-temperature asympotics. This example demonstrates clearly that distinct boundary conditions cause remarkable physical effects for quantum systems.

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1. Introduction

Quantum systems in less than three dimensions enjoy an increasing popularity and importance in physics. These seemingly simple systems (rings, boxes, "dots", etc.) exhibit unexpectedly interesting properties [1], many of which have originally been found in connection with quantum field theories. The recent developments in nanotechnology now make it possible to manufacture such quantum mechanical devices, allowing us to study these various features in laboratories [2–4]. With tunable control parameters — such as varying the magnetic flux that is driven through a ring, or influencing the parameters that characterize the boundary conditions at the walls of a box — these properties become governable, giving us thus controllable quantum devices that may be useful for many technological applications.

In fact, the dependence of the physical properties on the control parameters is quite strong. For example, the energy spectrum of a box or a ring with junctions changes considerably with different boundary/fitting conditions applied at the walls/junctions [5]. The aim of the present paper is to demonstrate a physical consequence of this effect in the context of quantum statistical mechanics. Namely, we show by the example of the box systems how different quantum statistical behavior emerges from distinct boundary conditions and the corresponding distinct spectra. One of the remarkable results is that not only the low-temperature behavior is sensitive to the difference in spectrum but also the high-temperature properties depend clearly on it.

The setting we consider is a one-dimensional quantum well/box, divided into two halves with an internal partition wall. Both halves contain the same number of noninteracting particles. We impose the same (Dirichlet) boundary conditions at the two ends of the box, while the boundary conditions at the two sides of the partition wall are chosen to be different (Dirichlet from the left, Neumann from the right). From the different emerging spectra in the two half regions, we calculate the quantum statistical force/pressure acting on the internal wall from the left and from the right, and the corresponding net force acting on it, as the function of temperature. We present both numerical results (which are obtained by appropriate truncations of the arising infinite sums) and analytical approximations, the latter ones aiming at understanding the low and the high temperature regimes.

The number of particles on both sides, N, is arbitrary, and is not necessarily macroscopically large. Our numerical results are presented for $N = 100$, which is a realistic population number in nanoscale quantum experiments [4]. The particles are considered as bosons in this paper, however, we mention that the results prove to be qualitatively (and partly quantitatively) similar for fermionic particles, too [6].

2. Low temperature regime

The system we consider is formulated as a one-dimensional quantum well of width $2l$ given by the interval $[-l, l]$ with a partition placed at the centre $x = 0$. At the end walls of the well the states are supposed to obey the Dirichlet boundary condition $\psi(\pm l) = 0$. At the centre, we assume that the partition imposes distinct boundary conditions on the left and the right, our choice is to impose the Dirichlet one for $x = -0$ and the Neumann one for $x = +0$:

$$\psi(-0) = 0, \qquad \psi'(+0) = 0. \tag{2.1}$$

The two half wells seperated by the partition then admit the energy levels $E_n^\pm = e_n^\pm \mathcal{E}$, $n = 1, 2, 3 \ldots$, with

$$e_n^+ = \left(n - \frac{1}{2}\right)^2, \qquad e_n^- = n^2, \qquad \mathcal{E} = \frac{\hbar^2}{2m}\left(\frac{\pi}{l}\right)^2. \tag{2.2}$$

Suppose that we put N identical bosonic particles into each of the two half wells. The particles will then distribute among the eigenstates according to the Bose-Einstein statistics,

$$N = \sum_n N_n^\pm, \qquad N_n^\pm = \frac{1}{e^{\alpha^\pm + b e_n^\pm} - 1}, \tag{2.3}$$

where we have introduced $b = \beta\mathcal{E}$ ($\beta = 1/kT$). Note that $\alpha^\pm$ are determined by the particle number constraint (the first of (2.3)) and are dependent on the temperature. The forces (or pressure) acting on the partition from the right and the left are then given by

$$F^\pm = -\sum_n \frac{\partial E_n^\pm}{\partial l} N_n^\pm. \tag{2.4}$$

For simplicity, in what follows we use the dimensionless force and temperature defined by

$$f^\pm = \frac{l}{2\mathcal{E}} F^\pm, \qquad t = \frac{1}{b} = \frac{k}{\mathcal{E}} T, \tag{2.5}$$

with which the net force on the partition becomes

$$\Delta f = f^- - f^+, \qquad f^\pm = \sum_n e_n^\pm N_n^\pm. \tag{2.6}$$

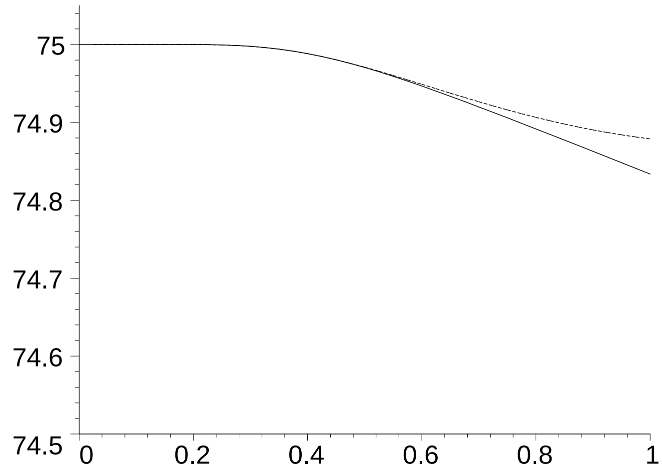

Figure 1. The net force $\Delta f(t)$ for $N = 100$, in the temperature region $t < 1$, obtained by a numerical computation (solid line), and approximated by Eq. (2.8) (dashed line).

Our objective is to find how the net force Δf behaves as a function of the temperature variable t.

To proceed, we first study the low temperature regime where a finite number of particles remain in the ground state $n = 1$. This occurs if $\alpha^\pm + be_1^\pm \ll 1$, and in this regime a numerical computation exhibits interesting behaviors of the net force Δf. Namely, as shown in Fig.1, Δf starts off by the value $\Delta f = 3N/4$ at $t = 0$ and decreases slightly but basically stays there for $t < 1$. Above $t \approx 1$ the net force starts to decrease almost linearly until it reaches its minimum at around $t \sim N$ (see Fig.2), and from there it increases to infinity. To see how these behaviors arise, let us consider the case of the extremely low temperatures $t < 1$, where most of the N particles are in the ground state. In this case, if we write $f^\pm$ in (2.6) as

$$f^\pm = e_1^\pm N + \sum_{n=2}^{\infty} g_n^\pm, \qquad g_n^\pm = \left(e_n^\pm - e_1^\pm\right) N_n^\pm, \tag{2.7}$$

then we find that the first term gives the zero temperature value $f^\pm(0)$ and the rests represent the corrections from the higher energy levels at finite temperatures. Since $N_n^\pm$ decreases exponentially fast for higher n, we may keep only the first contribution $n = 2$ to get

$$\Delta f(t) \approx \frac{3}{4}N + (3\,e^{-3/t} - 2\,e^{-2/t}). \tag{2.8}$$

This gives a good approximation for $t < 1$ as seen in Fig.1.

The linear decrease of the net force observed for temperatures higher (but not much higher) than $t = 1$ may be understood heuristcially as follows. First, we classify the energy levels into three categories, where the first is those levels for which $b(e_n^{\pm} - e_1^{\pm}) \ll 1$, the second is those for which $b(e_n^{\pm} - e_1^{\pm}) \gg 1$, and the third is the rest, *i.e.*, those for which $b(e_n^{\pm} - e_1^{\pm})$ is not far from 1. Let m be the level whose $b(e_n^{\pm} - e_1^{\pm})$ is closest to 1, that is, $b(e_m^{\pm} - e_1^{\pm}) \approx 1$. Levels with $n \ll m$ thus belong to the first category, and for these one has $\alpha^{\pm} + be_n^{\pm} \approx b(e_n^{\pm} - e_1^{\pm})$ and hence $N_n^{\pm} \approx \frac{1}{b(e_n^{\pm} - e_1^{\pm})}$. The corresponding $g_n^{\pm}$ given in (2.7) are then found to be $g_n^{\pm} \approx \frac{1}{b}$. Thus we have $g_n^- - g_n^+ \approx 0$ showing that the levels in this category do not contribute to the net force. On the other hand, levels with $n \gg m$ belong to the second category, and for these we have $N_n^{\pm} \approx e^{-b(e_n^{\pm} - e_1^{\pm})}$ but since $b(e_n^{\pm} - e_1^{\pm}) \gg 1$, the corresponding force F_n is seen to be exponentially small and can be ignored. Thus the contribution to the net force can comes only from the intermediate levels belonging to the third category. As a representative, let us choose m such that $b(e_m^+ - e_1^+) = 1$ holds in effect, which is equivalent to $m^2 - m = t$, for the right half well. Since we have $N_m^+ = 1/(e-1)$, we get

$$g_m^+ = \frac{1}{b} \cdot \frac{1}{e-1}. \tag{2.9}$$

In contrast, for the level m for the left half well, we have $b(e_m^- - e_1^-) = \frac{m^2-1}{t} = 1 + \frac{1}{m}$ and hence $N_m^- = 1/(e^{1+1/m} - 1)$. Thus the contribution to the force becomes

$$g_m^- = \frac{1}{b} \cdot \frac{1 + \frac{1}{m}}{e^{1+1/m} - 1}. \tag{2.10}$$

Combining (2.9) and (2.10), and estimating roughly that the total number of levels in the third category is of the order of m, ranging from $m/2 < n < 3m/2$, say, we just multiply the number m to each of the contribution to find

$$\Delta f(t) \approx \frac{3}{4}N + \sum_{n=m/2}^{3m/2} (g_n^- - g_n^+) = \frac{3}{4}N - \frac{t}{(e-1)^2}. \tag{2.11}$$

The linear decrease of the net force is now seen in (2.11). Our argument assumes $\alpha^{\pm} + be_1^{\pm} < b(e_n^{\pm} - e_1^{\pm})$ which gives the upper limit of the temperature t for which the heuristic formula (2.11) is available. The numerical result shows that the limit is around $t \approx 2N/3$.

If the temperatures are even higher $t \gg 1$ but still satisfy $\alpha^{\pm} + be_1^{\pm} \ll 1$ remaining in the low temperature regime, the above approximation becomes worse and we need to resort to more systematic means to reproduce the numerical results. One such method valid for

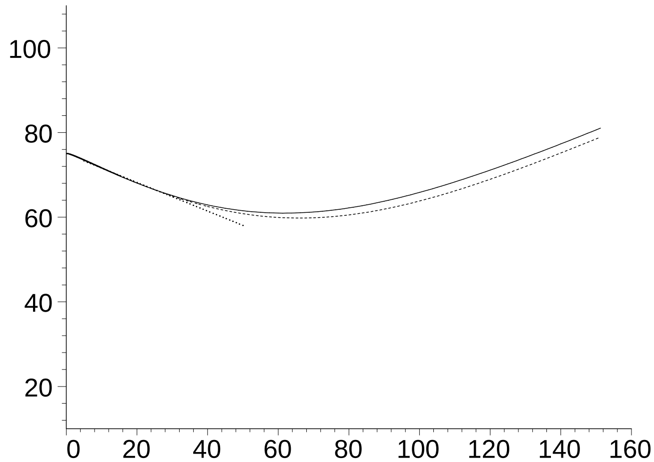

Figure 2. The net force $\Delta f(t)$ for $N = 100$ and in the temperature region $0 < t < 160$, obtained by a numerical computation (solid line), and approximated by Eq. (2.11) (dotted line), and by Eq. (2.16) using Eq. (2.18) (dashed line).

$t \gg 1$ is to consider the infinite sums as the trapezoidal approximations of corresponding integrals. Thus we can write

$$\sum_{n=1}^{\infty} y(s_n) \approx \frac{y(s_1)}{2} + \frac{1}{\Delta s}\int_{s_1}^{\infty} y(s)\mathrm{d}s \tag{2.12}$$

for functions $y(s)$ vanishing at infinity, $\lim_{s\to\infty} y(s) = 0$. The summation in (2.12) is taken at equidistant points, s_n, $n = 1, 2, \ldots$, with $\Delta s = s_{n+1} - s_n =$ constant, and obviously the approximation is better for smaller Δs. Using this approximation, we obtain

$$\begin{aligned} f^{\pm} &= \frac{1}{b}\sum_{n=1}^{\infty} \frac{be_n}{\mathrm{e}^{\alpha^{\pm}+be_n^{\pm}} - 1} = -\frac{N\alpha^{\pm}}{b} + \frac{1}{b}\sum_{n=1}^{\infty} \frac{\alpha^{\pm} + (s_n^{\pm})^2}{\mathrm{e}^{\alpha^{\pm}+(s_n^{\pm})^2} - 1} \\ &\approx -\frac{N\alpha^{\pm}}{b} + \frac{1}{b}\left[\frac{1}{2}\frac{\alpha^{\pm} + (s_1^{\pm})^2}{\mathrm{e}^{\alpha^{\pm}+(s_1^{\pm})^2} - 1} + \frac{1}{\sqrt{b}}\int_{s_1^{\pm}}^{\infty} \frac{\alpha^{\pm} + s^2}{\mathrm{e}^{\alpha^{\pm}+s^2} - 1}\mathrm{d}s\right], \end{aligned}$$

where we have introduced $s_n^{\pm} = \sqrt{be_n^{\pm}}$ which are equidistant on account of (2.2). Note that the increments $\Delta s^{\pm} = \sqrt{b} = 1/\sqrt{t}$ are indeed small for $t \gg 1$. Since $\frac{z}{\mathrm{e}^z - 1} \approx 1$ for small z, we can approximate the second term by $\frac{1}{2b}$, and similarly the integral $\int_0^{s_1^{\pm}} \frac{\alpha^{\pm}+s^2}{\mathrm{e}^{\alpha^{\pm}+s^2}-1}\mathrm{d}s$ by $s_1^{\pm}$. We thus obtain

$$f^{\pm} \approx \frac{-N\alpha^{\pm} + 1/2 - s_1^{\pm}/\sqrt{b}}{b} + \frac{1}{b^{3/2}}\int_0^{\infty} \frac{\alpha^{\pm} + s^2}{\mathrm{e}^{\alpha^{\pm}+s^2} - 1}\mathrm{d}s\,. \tag{2.13}$$

Employing the formula $\frac{z}{\mathrm{e}^z-1} \approx \mathrm{e}^{-z}\left(1+\frac{z}{2}+\frac{z^2}{12}\right)$ which is handy for evaluating the integral approximately, we find

$$\int_0^\infty \frac{\alpha^\pm + s^2}{\mathrm{e}^{\alpha^\pm + s^2}-1}\mathrm{d}s \approx \frac{\sqrt{\pi}}{96}(63-35\alpha^\pm) + \mathcal{O}\left(\alpha^{\pm 2}\right), \tag{2.14}$$

and hence

$$f^\pm \approx \left(-N\alpha^\pm + 1/2 - \sqrt{e_1^\pm}\right)t + \frac{\sqrt{\pi}}{96}(63-35\alpha^\pm)\,t^{3/2}\,. \tag{2.15}$$

The net force is then

$$\Delta f \approx \left(Nt + \frac{35}{96}\sqrt{\pi}\,t^{3/2}\right)(\alpha^+ - \alpha^-) + \left(\sqrt{e_1^+} - \sqrt{e_1^-}\right)t\,. \tag{2.16}$$

In passing we remark that this formula (2.16) turns out to be valid even for small temperatures. This can be seen, for example, by considering the $t \to 0$ limit, where $N_1^\pm \approx N$ and hence from (2.3) we have $\alpha^\pm \approx \ln(1+1/N) - be_1^\pm$. Thus the net force (2.16) is found to be $\Delta f \approx N\left(e_1^- - e_1^+\right) = 3N/4$ for $t \ll 1$ as seen in (2.8).

To make use of (2.16), we need to determine the $\alpha^\pm$ as functions of t from the total number costraint in (2.3). This can be done with the help of the same approximation method as used above. Namely, upon using (2.12) we write down the constraint condition as

$$\begin{aligned} N &= \sum_{n=1}^\infty N_n^\pm = N_1^\pm + \sum_{n=2}^\infty \frac{1}{\mathrm{e}^{\alpha^\pm + be_n^\pm}-1} \\ &\approx \frac{1}{\mathrm{e}^{\alpha^\pm + be_1^\pm}-1} + \frac{1/2}{\mathrm{e}^{\alpha^\pm + be_2^\pm}-1} + \frac{1}{\sqrt{b}}\int_{s_2^\pm}^\infty \frac{\mathrm{d}s}{\mathrm{e}^{\alpha^\pm + s^2}-1}, \end{aligned} \tag{2.17}$$

where we have kept $N_1^\pm$ separately to achieve a better approximation (since $N_n^\pm$ are rapidly decreasing functions of n for small n). Limiting the range of integration to $[0, \sqrt{2}]$ which provides the main contribution to the integral, and using $\frac{1}{\mathrm{e}^z-1} \approx \frac{1}{z} - \frac{1}{2}$ valid on the range, we find

$$\begin{aligned} N &\approx \frac{1}{\alpha^\pm + be_1^\pm} + \frac{1/2}{\alpha^\pm + be_2^\pm} - \frac{3}{4} - \frac{1}{\sqrt{b}}\frac{\sqrt{2-\alpha^\pm} - s_2^\pm}{2} \\ &\quad + \frac{1}{\sqrt{b|\alpha^\pm|}}\left[A\left(\frac{\sqrt{|\alpha^\pm|}}{s_2^\pm}\right) - A\left(\frac{\sqrt{|\alpha^\pm|}}{\sqrt{2-\alpha^\pm}}\right)\right], \end{aligned} \tag{2.18}$$

where the function A is the $\arctan$ function for positive $\alpha^\pm$, and is the $\operatorname{arctanh}$ function for negative $\alpha^\pm$. Unfortunately, it is not easy to solve (2.18) directly for $\alpha^\pm$ even approximately to obtain an analytic formula that can be used in (2.16) to reproduce the numerical result. Nevertheless, the formula (2.18) has allowed us to evaluate the infinite sum to a good

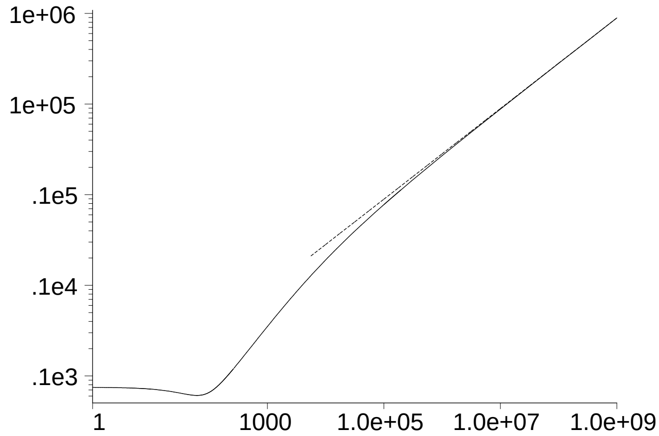

Figure 3. The net force $\Delta f(t)$ for $N = 100$, obtained by a numerical computation (solid line), and approximated for high temperatures with Eq. (3.7) (dashed line).

accuracy, and we can solve (2.18) indirectly for $\alpha^{\pm}$ by numerical means. The outcome of this semi-analytic analysis is in good agreement with the numerical computation as shown in Fig.2.

3. High temperature regime

Let us now determine the high-temperature asymptotic behavior of the net force. For increasing temperature, we expect $N_1^{\pm}$ to decrease so [see (2.3) for $n = 1$] we expect $\alpha^{\pm}$ to increase to higher positive values. Inspired by this, let us expand $N_n^{\pm}$ in $q^{\pm} := \mathrm{e}^{-\alpha^{\pm}}$ as

$$N_n^{\pm} = \frac{q^{\pm}\mathrm{e}^{-be_n^{\pm}}}{1 - q^{\pm}\mathrm{e}^{-be_n^{\pm}}} = \sum_{k=1}^{\infty}(q^{\pm})^k \mathrm{e}^{-kbe_n^{\pm}}\,, \tag{3.1}$$

which is valid for any positive $\alpha^{\pm}$. Thus

$$N = \sum_{n=1}^{\infty} N_n^{\pm} = \sum_{k=1}^{\infty}(q^{\pm})^k \sum_{n=1}^{\infty} \mathrm{e}^{-kbe_n^{\pm}} = \sum_{k=1}^{\infty}(q^{\pm})^k \left[-\frac{\sigma^{\pm}}{2} + \frac{1}{2}\sum_{n=-\infty}^{\infty} \mathrm{e}^{-kbe_n^{\pm}}\right], \tag{3.2}$$

with the constants $\sigma^{+} = 0$, $\sigma^{-} = 1$ corresponding to the $\pm$ half wells, where we have extended the meaning of the notation $e_n^{\pm}$ [see (2.2)] to negative ns, too. Applying now the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} y(n) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}s\, y(s)\, \mathrm{e}^{2\pi i m s}\,, \tag{3.3}$$

we obtain

$$N=\sum_{k=1}^{\infty}(q^{\pm})^k\left[-\frac{\sigma^{\pm}}{2}+\sqrt{\frac{\pi}{4kb}}\sum_{m=-\infty}^{\infty}(\tau^{\pm})^m\mathrm{e}^{-\frac{\pi^2}{kb}m^2}\right] \tag{3.4}$$

with $\tau^{\pm}=\mp 1$. Similarly, for the force $f^{\pm}$, one can find

$$f^{\pm}=\sum_{n=1}^{\infty}e_n^{\pm}N_n^{\pm}=\sum_{k=1}^{\infty}(q^{\pm})^k\sqrt{\frac{\pi}{16k^3b^3}}\sum_{m=-\infty}^{\infty}(\tau^{\pm})^m\left(1-\frac{2\pi^2}{kb}m^2\right)\mathrm{e}^{-\frac{\pi^2}{kb}m^2}\,. \tag{3.5}$$

For the high-temperature asymptotic behavior ($q^{\pm}\to 0$), it suffices to consider only the first some terms in the sums over k [both in (3.4) and (3.5)], and within each term to keep only the $m=0$ term in the sums over m (the $m\neq 0$ terms being exponentially suppressed). Now, the leading, $k=1$ term in (3.4) gives that $q^{\pm}=2N\left(\frac{b}{\pi}\right)^{1/2}+\mathcal{O}\left(b\right)$. Since this leading behavior of $q^{\pm}$ is independent of $\sigma^{\pm}$, inserting it into (3.5) gives that the leading, $\mathcal{O}\left(b^{-1}\right)$ term of $f^{\pm}$ (coming from $k=1$, $m=0$) is also σ-independent. Hence, this term will drop out from the net force. Therefore, to have the first nonvanishing term in the net force we need the first subleading term in q, too. Incorporating the $k=2$ term as well for $q^{\pm}$, we find

$$q^{\pm}=2N\left(\frac{b}{\pi}\right)^{1/2}+2N\left[\sigma^{\pm}-\sqrt{2}N\right]\frac{b}{\pi}+\mathcal{O}\left(b^{3/2}\right)\,. \tag{3.6}$$

Plugging this into (3.5) and then calculating the net force yields

$$\Delta f=\frac{N}{2}\left(\frac{t}{\pi}\right)^{1/2}+\mathcal{O}\left(t^{0}\right)\,. \tag{3.7}$$

We can see in Fig.3 how the net force actually reaches this square-root asymptotic behavior at high temperatures.

4. Discussion

We have found that the net force acting on the separating wall is nonzero at low temperatures, being practically constant for very small temperatures and starting to decrease when temperature is increased. Knowing that the energy spectrum is different on the two halves this property is not very surprising. What is surprising, however, is that this decrease stops at a certain temperature and the net force starts to increase above this value. Furthermore, a remarkable fact is that this increase does not stop nor converges to some finite high-temperature limit but increases to infinity, as the square root of the temperature. From the naive expectation that such quantum effects coming from the different boundary conditions should vanish at high temperatures where the classical picture would be available, this result seems quite unusual. However, this may be understood by the fact that, contrary to most quantum systems, one dimensional boxes have such energy spectra that the level spacing is not decreasing but increasing for higher energy levels (which is actually valid not only for boxes with Dirichlet and/or Neumann boundary conditions but for all other boxes as well [5]). In other words, quantum boxes can be distinguished by their high-temperature behavior, too.

We mention that the calculation presented here could be repeated for boxes with other boundary conditions, too. We note however that, for most box systems, the energy values are determined by a transcendental equation [5], and hence a certain additional difficulty for carrying out the calculations, especially the analytical ones, will arise there.

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