Abstract The closed-form expression for the quantum partition function of the improved Tietz oscillator is obtained using the Voronoi summation formula.

Keywords Tietz potential, oscillator, vibrational, quantum, partition function

1. The aim of [1] was to obtain closed-form expression for the quantum vibrational partition function for the improved Tietz potential energy model [2]. According to [1] the terms with \( m \neq 0 \) include the quantum corrections in following equation

\[
\sum_{n=0}^{N} f(n) = \frac{1}{2} [f(0) - f(N + 1)] + \int_{0}^{\infty} f(x) \exp(-i2\pi n x) dx ,
\]  

where \( i \) is the imaginary unit. Neglecting the quantum corrections Eq. 1 was represented in [1] as

\[
\sum_{n=0}^{N} f(n) = \frac{1}{2} [f(0) - f(N + 1)] + \int_{0}^{\infty} f(x) dx .
\]  

But neglecting the quantum corrections contradicts to the aim of [1] (Eqs. 1-2 are equivalent to Eqs. 9-10 [1]).

Eq. 11 [1] for the partition function was obtained using Eq. 2. As one can see Eq. 11 [1] takes into account the vibrational quantum states. This is the second contradiction in [1].

According to [1] Eq. 1 is the Poisson summation formula (PSF). PSF does not consider the quantum corrections [4]. Therefore the terms with \( m \neq 0 \) in Eq. 1 does not include the quantum corrections. This is the third contradiction in [1].

There is no a proof in [1] that the terms with \( m \neq 0 \) in Eq. 1 include the quantum corrections to the classical partition function.

So, there is the inner inconsistency in [1].

2. The Poisson summation formula is valid if \( \int_{-\infty}^{\infty} |f(x)| dx < \infty \) [4]. One can see that

\[
\int_{-\infty}^{\infty} |f(v)| dv = \infty \quad \text{for} \quad f(v) = \exp(-E_v / kT) , \quad \text{where} \quad k \quad \text{is the Boltzmann constant,} \quad T \quad \text{is the temperature} \quad \text{and the energy} \quad E_v \quad \text{of} \quad v-\text{th vibrational quantum level} \quad \text{is defined from Eq. 2 [1]}. 
\]

Therefore Eqs. 1-2 cannot be used to calculate the partition function \( Q = \sum_{v=0}^{N} \exp(-E_v / kT) \), where \( N \) is the number of exited bonded states.

3. Eq. 2 can be represented as

\[
\int_{0}^{\infty} f(x) dx = \sum_{n=0}^{N} \frac{1}{2} [f(n) + f(n + 1)] .
\]  

(3)
It is easy to establish that Eq. 3 is equivalent to

$$\int_0^a f(x)dx = \sum_{n=0}^{a/\Delta - 1} \frac{1}{2} [f(n\Delta) + f((n+1)\Delta)] ,$$

(4)

where $\Delta = 1$ and $a = (N+1)\Delta$. One can see that Eq. 4 is correct if $f(x)$ is a linear function or it is equal to a constant [3].

According to the trapezoid rule [3]

$$\int_0^a f(x)dx = \sum_{n=0}^{a/\Delta - 1} 0.5 \cdot [f(n \cdot \Delta) + f((n+1)\Delta)] \bigg|_{\Delta \to 0} .$$

(5)

We conclude from the comparison of Eqs. 4 and 5 that Eq. 4 is incorrect for a non-linear function $f(x)$. Hence Eqs. 2-3 are incorrect for a non-linear function $f(x)$.

One can conclude from above comments 2 and 3 that Eqs. 11 [1] and the closed-form expressions (Eqs. 14-16 [1]), obtained in [1] using Eq. 2 for the partition function, are incorrect. Eqs. 14-16 [1] are main results of [1].

4. The function $f(v) = \exp(-E_v / kT)$ is the non-linear function of $v$. Eq. 2 is incorrect for a non-linear function $f(v)$. Therefore Eqs. 11 and 14-16 [1] are incorrect.

5. Fig. 2 [1] confirms the incorrectness of Eq. 14 [1] for the partition function of CO molecule.

6. One can conclude on the basis of above comments 1-5 that the conclusions [1] based on the incorrect Eqs. 14-16 [1] could be incorrect.

There exists the exact Voronoi summation formula

$$\sum_{n=0}^{N} f(n) = \int_0^a f(x)dx + 2 \sum_{m=1}^{\infty} \int_0^a f(x) \cos(2\pi mx)dx$$

(6)

for smooth function $f(x)$ of bonded variation [5-7] which cannot obey the condition

$$\int_{-\infty}^{\infty} |f(x)|dx < \infty .$$

Eq. 6 can be represented as

$$\sum_{n=0}^{N} f(n) = \sum_{m=\infty}^{-\infty} \int_{m}^{m} f(x) \exp(-i2\pi mx)dx .$$

(7)

Comparing Eqs. 1 and 7 one can conclude that Eq. 1 is incorrect.

If we neglect in Eq. 6 the terms with $m \neq 0$ as it was done in [1] then using

$$\sum_{n=0}^{N} f(n) = \int_0^a f(x)dx$$

and repeating the mathematical operations done in [1] we obtain

$$Q = \int_0^{v_{\text{max}}} e^{-\beta \left[ D_v - \frac{1}{2} \left( \frac{D_1}{v + D_2} \frac{x + D_3}{2} \right)^2 \right]} dx$$

instead of the incorrect Eq. 11 [1]. One can easily see that:
- the upper limit $v_{\text{max}} + 1$ must be replaced by $v_{\text{max}}$ in the integral in left hand side of Eq. 12 [1];
- it is necessary to replace $v_{\text{max}}$ by $v_{\text{max}} - 1$ in Eqs. 18, 20 and 21 [1];
- the term \( e^{\beta b_1^2} - e^{\beta b_2^2} \) in the square brackets in the right hand sides of Eqs. 14 and 16 [1] must be removed, and therefore Eq. 15 [1], which is the power series of Eq. 14 for \( \beta \ll 1 \), is incorrect;
- it is necessary to use the correct relation \( b_2 = \frac{\delta_1}{v_{\text{max}} + \delta_2} - \frac{v_{\text{max}} + \delta_2}{2} \) instead of the incorrect one
\[
b_2 = \frac{\delta_1}{v_{\text{max}} + 1 + \delta_2} - \frac{v_{\text{max}} + 1 + \delta_2}{2}
\]
in Eqs. 12, 14 and 15 [1];
- it is necessary to use the correct relation \( c_v = e^{a(v_{\text{max}} - b)v_{\text{max}}} \) in Eq. 21 [1] instead of incorrect one \( c_v = e^{a(v_{\text{max}} + 1)^2 - b(v_{\text{max}} + 1)} \).

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