The tau-oscillator

2002 J. Phys. A: Math. Gen. 35 L591

(http://iopscience.iop.org/0305-4470/35/42/101)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) L591–L595 PII: S0305-4470(02)37972-1

LETTER TO THE EDITOR

The tau-oscillator

Viorel Badescu[1] **and Peter T Landsberg**[2]

[1] Candida Oancea Institute of Solar Energy, Polytechnic University of Bucharest, Spl Independentei 313, Bucharest 79590, Romania
[2] Faculty of Mathematical Studies, University of Southampton, Southampton SO17 1BJ, UK

E-mail: badescu@theta.termo.pub.ro and P.T.Landsberg@maths.soton.ac.uk

Received 11 June 2002
Published 8 October 2002
Online at stacks.iop.org/JPhysA/35/L591

Abstract
The tau-oscillator is a one-dimensional quantum-mechanical oscillator which can exist only below a critical temperature $T_{\max}$. Its quantized energy levels have the usual form but, unusually, these degeneracies involve the energy levels. A generalized equipartition law is also found and the constant volume heat capacity can exhibit a Schottky anomaly.

PACS numbers: 05.20.−y, 05.30.−d

Most physical systems cannot exist above a certain characteristic temperature. At this temperature some constituent chemical may decompose, a phase change may occur, a new chemical reaction may be initiated, etc. We have sought to study this situation from the point of view of basic physics but to our surprise have found no relevant literature. As an example we took the one-dimensional quantum-mechanical oscillator and present the results below.

One knows that a thermodynamic function may, with only minor additional assumptions, determine the energy level spectrum of a system. This is shown explicitly starting from the energy variance in the case of the 1D harmonic oscillator. One can also start with its entropy expression ([1], section 16.4, [2]).

Now proceed to the case when there is a maximum temperature $T_{\max}$ at which this oscillator can exist. We shall call this system a tau-oscillator. Tau is a reminder of the importance of the temperature for this system.

Recall that for N identical one-dimensional quantum-mechanical oscillators the energy variance σ_E^2 per particle equals the square of the mean energy per particle, reduced by the square of the zero-point or ground-state energy level, E_{gs}^2. Also, with $\beta \equiv 1/kT$,

$$\sigma_E^2 = -\left(\frac{\partial U}{\partial \beta}\right)_{V,N} \tag{1}$$

([1], equation (16.3)) where U is the average energy per particle and V the volume of the system. It follows that

$$\mathrm{d}\beta = \frac{\mathrm{d}U}{E_{\mathrm{gs}}^2 - U^2}. \tag{2}$$

Our key assumption is now that the system cannot exist above a maximum temperature $T_{\max}$, giving rise to

$$\beta_{\min} \equiv \frac{1}{kT_{\max}} \qquad \text{and} \qquad \Delta\beta \equiv \beta - \beta_{\min}.$$

Then there is a maximum mean energy per particle $U_{\max}$ of the system. After some algebra an integration of (2) yields

$$U = E_{\mathrm{gs}} \frac{\exp(2E_{\mathrm{gs}}\Delta\beta) + r}{\exp(2E_{\mathrm{gs}}\Delta\beta) - r} \tag{3}$$

$$r \equiv \frac{U_{\max} - E_{\mathrm{gs}}}{U_{\max} + E_{\mathrm{gs}}} > 0. \tag{4}$$

When $T \to T_{\max}$, $\beta \to \beta_{\min}$, $\Delta\beta \to 0$ and $U \to U_{\max}$, as expected.

We now use the standard result

$$U = -\left(\frac{\partial \ln Z}{\partial\beta}\right)_{V,N} = -\left(\frac{\partial \ln Z}{\partial\Delta\beta}\right)_{V,N} \tag{5}$$

where Z is the canonical partition function. This integration to obtain Z, though elementary, involves some lines of algebra, and yields

$$Z = \frac{Z_0 \exp(E_{\mathrm{gs}}\Delta\beta)}{\exp(2E_{\mathrm{gs}}\Delta\beta) - r} \tag{6}$$

where Z_0 is a constant of integration. Expanding $1/[\exp(2E_{\mathrm{gs}}\Delta\beta) - r]$ of equation (6) in a Taylor series, one finds

$$Z = \sum_{n=0}^{\infty} Z_0 r^n \exp\left[-2E_{\mathrm{gs}}\left(n + \frac{1}{2}\right)\Delta\beta\right] \equiv \sum_{n=0}^{\infty} g_n \exp(-\beta E_n). \tag{7}$$

We learn from this that the tau-oscillator, which has a zero-point energy E_{gs} and exists only below a maximum temperature $T_{\max}$, has the following energy levels and degeneracies:

$$E_n = 2E_{\mathrm{gs}}\left(n + \tfrac{1}{2}\right) \tag{8}$$

and

$$g_n \equiv Z_0 r^n \exp(\beta_{\min} E_n) \qquad (n = 0, 1, \ldots). \tag{9}$$

The degeneracy is unusual in that it is not an integer, and it is unexpected in that it involves the energy levels.

Simple calculations prove that the usual argument leading from the Lagrangian multiplier β to $1/kT$ and to equations (1) and (5) is not affected by the fact that β has a limited range of existence.

One obtains a new equipartition law, i.e. the law for the tau-oscillator, by passing to the limit $E_{\mathrm{gs}} \to 0$ in equations (3) and (4). One finds

$$\lim_{E_{\mathrm{gs}} \to 0} U = \frac{kT}{1 - \frac{T}{T_{\max}}}. \tag{10}$$

Of course, in the usual case $T_{\max} \to \infty$ the normal equipartition law is found from (10).

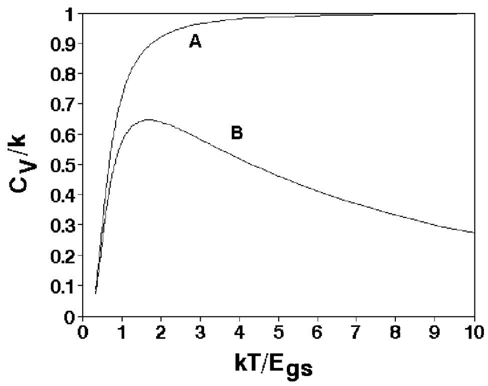

Figure 1. Constant volume heat capacity as a function of temperature for two systems of different quantum tau-oscillators. Curve A applies to a tau-oscillator close to the usual quantum oscillator ($\frac{E_{gs}}{U_{max}} = 10^{-8}$ and $\frac{E_{gs}}{kT_{max}} = 10^{-8}$). Curve B applies to a tau-oscillator far from usual conditions ($\frac{E_{gs}}{U_{max}} = 0.1$ and $\frac{E_{gs}}{kT_{max}} = 0.01$). The usual quantum oscillator corresponds to $U_{max} \to \infty$, $T_{max} \to \infty$.

Table 1. Internal energy U and constant volume heat capacity C_V for various oscillators.

System	U	$C_V \equiv \frac{\partial U}{\partial T}$
1. Classical oscillator ($E_{gs} = 0$, $T_{max} \to \infty$)	$\frac{1}{\beta} = kT$	k
2. Classical tau-oscillator ($E_{gs} = 0$, $T_{max} < \infty$)	$\frac{kT}{1-\frac{T}{T_{max}}}$	$\frac{k}{(1-\frac{T}{T_{max}})^2}$
3. Quantum oscillator ($E_{gs} > 0$, $T_{max} \to \infty$)	$E_{gs}\frac{\exp(2E_{gs}\beta)+1}{\exp(2E_{gs}\beta)-1}$	$k\frac{4E_{gs}^2\beta^2 \exp(2E_{gs}\beta)}{[\exp(2E_{gs}\beta)-1]^2}$
4. Quantum tau-oscillator ($E_{gs} > 0$, $T_{max} < \infty$)	$E_{gs}\frac{\exp(2E_{gs}\Delta\beta)+r}{\exp(2E_{gs}\Delta\beta)-r}$	$k\frac{4E_{gs}^2\beta^2 r \exp(2E_{gs}\Delta\beta)}{[\exp(2E_{gs}\Delta\beta)-r]^2}$

Another special case is found from (9) in the limit of the usual quantum oscillator:

$$T_{max} \to \infty \qquad \beta_{min} \to 0 \qquad r \to 1 \qquad \text{and} \qquad g_n \to Z_0.$$

Table 1 summarizes formulae for the internal energy and the constant volume heat capacity $C_V \equiv \frac{\partial U}{\partial T}$ for various classical and quantum oscillators. Simple algebra proves that when applied to U, the operators $\frac{\partial}{\partial T}$ and $\lim_{E_{gs}\to 0}$ commute for the usual quantum oscillator but do not commute for the quantum tau-oscillator.

Figure 1 shows the dependence of C_V on temperature for two tau-oscillator systems. Curve A applies to a tau-oscillator close to the usual quantum oscillator while curve B refers to a tau-oscillator far from usual conditions. The maximum of C_V in the case B is similar to the so-called Schottky anomalies in the heat capacity due to internal freedom degrees activated by magnetic fields and other causes (see figure 14 of [3] for instance). Conditions for the occurrence of a local maximum in the heat capacity of tau-oscillators are briefly explained below. One uses the following notation:

$$x \equiv E_{gs}\beta = \frac{E_{gs}}{kT} \qquad x_{min} = E_{gs}\beta_{min} = \frac{E_{gs}}{kT_{max}}. \tag{11}$$

Using (11) in table 1 row four yields

$$\frac{C_V}{k} = \frac{4x^2 r \exp[2(x - x_{\min})]}{\{\exp[2(x - x_{\min})] - r\}^2}. \tag{12}$$

To obtain a local maximum for the heat capacity one computes $\frac{\mathrm{d}\left(\frac{C_V}{k}\right)}{\mathrm{d}x} = 0$ and from (12) one finds

$$\frac{1-x}{1+x} \exp[2(x - x_{\min})] = r < 1. \tag{13}$$

Solving equation (13) in the unknown x will determine that value $\tilde{x}$ where the heat capacity is a maximum (say $C_{V,\max}$). One can see that $x_{\min} < \tilde{x} < 1$. The last inequality applies because $r > 0$ in (13). The lhs of equation (13) is a monotonous decreasing function of x and a solution exists if

$$\frac{1-x_{\min}}{1+x_{\min}} \exp[2(x_{\min} - x_{\min})] > r. \tag{14}$$

Using (4) and (11) one finds that (14) requires

$$\frac{E_{\mathrm{gs}}}{U_{\max}} > \frac{E_{\mathrm{gs}}}{kT_{\max}} \qquad \text{and} \qquad kT_{\max} > U_{\max}. \tag{15}$$

When equation (15) is fulfilled (case of curve B in figure 1) the heat capacity has a maximum. Otherwise, it has a monotonous variation as a function of temperature (case of curve A in figure 1).

Now, let us suppose equation (15) is fulfilled. Then the solution $\tilde{x}$ of equation (13) verifies, of course,

$$\frac{1-\tilde{x}}{1+\tilde{x}} \exp[2(\tilde{x} - x_{\min})] = r. \tag{13$'$}$$

Use of (13′) in (12) gives the maximum heat capacity as follows:

$$\frac{C_{V,\max}}{k} = \frac{1}{\tilde{x}} - \tilde{x} \tag{16}$$

$C_{V,\max}$ has a monotonous dependence on $\tilde{x}$. When $\tilde{x}$ varies between $x_{\min}$ and 1, $C_{V,\max}$ varies between $\frac{1}{x_{\min}} - x_{\min}$ and 0. One can see that $C_{V,\max}/k$ can be larger or smaller than the unity as follows:

$$\tilde{x} < \tilde{x}_{\mathrm{cr}} \quad \Rightarrow \quad \frac{C_{V,\max}}{k} > 1 \tag{17a}$$

$$\tilde{x} > \tilde{x}_{\mathrm{cr}} \quad \Rightarrow \quad \frac{C_{V,\max}}{k} < 1 \tag{17b}$$

where the critical value $\tilde{x}_{\mathrm{cr}}$ (related to the critical temperature T_{cr}) is incidentally given by the golden section

$$\tilde{x}_{\mathrm{cr}} \equiv \frac{E_{\mathrm{gs}}}{kT_{\mathrm{cr}}} = \frac{\sqrt{5}-1}{2} \tag{18}$$

($\tilde{x}_{\mathrm{cr}}$ is obtained by making $\frac{C_{V,\max}}{k} = 1$ in equation (16)). We conclude that there is a possibility of a very sharp maximum, under the condition (17a) above and $\tilde{x}$ very close to $x_{\min}$ in equation (16), as already noted in the case of Schottky anomalies [3].

Our study is theoretically based and to link the results to specific experiments is a major task best left to the people who have conducted these experiments, of which there are plenty. We enumerate below a few systems showing specific heat maximas:

1. Helium-4 confined to a 9869 A planar geometry [4].
2. The heat capacity of erbium exhibits a maximum near 18.7 K. This is presumed to be due to an antiferromagnetic to ferromagnetic phase transition [5].
3. A heat capacity maximum due to magnetic short-range order was observed at 1.4 K in an organic spin-1 Kagome antiferromagnet [6].
4. An excess specific heat maximum occurred at 307.7 K in a colloidal microgel system [7].

The fact that there are so many examples of specific heat maxima does suggest the desirability of having a general theory of the type we are proposing. Extensions of this work to Fermi and Bose systems are being prepared for publication.

Acknowledgments

The authors thank the referee for useful comments. P T Landsberg is indebted for support to NATO under contract PST.CLG.975758.

References

[1] Landsberg P T 1990 *Thermodynamics and Statistical Mechanics* (New York: Dover)
[2] Landsberg P T 1981 *Eur. J. Phys.* **2** 208
[3] Kittel C 1971 *Introduction to Solid State Physics* 4th edn (New York: Wiley) ch 15 problem 5
[4] Kimball M O and Gasperini F M 2000 *Physica* B **284** 47
[5] Pecharsky V K, Gschneidner K A Jr and Fort D 1993 *Phys. Rev.* B **47** 5063
[6] Wada N, Kobayashi T, Yano H, Okuno T, Yamaguchi A and Awaga K 1997 *J. Phys. Soc. Japan* **66** 961
[7] Murray M, Rana F, Haq I, Cook J, Chowdhry B Z and Snowden M J 1994 *J. Chem. Soc. Chem. Commun.* 1803