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by

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ABSTRACT

The quantum single one-dimensional oscillator associated with a potential proportional to $|x|^{\nu}$ ($\nu > 0$) is discussed. The exact energy eigenvalues recently established by Turschner are further elaborated and convenient exact as well as asymptotic relations are exhibited. The exact $T \to 0$ and $T \to \infty$ specific heat is discussed and numerical results for typical values of ν and intermediate temperatures are presented.

I - INTRODUCTION

There are very few quantum systems on which exact quantitative knowledge is available. In what concerns the energy eigenvalues, since the 1979 Turschner paper[1], we can presently include among them single oscillator associated with the Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\left\{p^2 + a^{\left(\frac{\nu+2}{2}\right)}|x|^{\nu}\right\} \quad (a,\nu > 0) \tag{1}$$

Approximate calculations of the corresponding eigenvalues have been performed for $\nu = 4$[2,3] and $\nu = 6,8$[4] (for comparison purposes, we come back onto these works later on). The exact result is now available[1]; however Turschner provided it in a form which is not appropriate for operational purposes. In the present work we further elaborate his result and achieve an operationally convenient explicit form, as well as useful recursive relations. This is done in Section II.

Once the exact energy spectrum is known, it is natural to seek for the calculation of the partition function and consequently the specific heat. As matter of fact, for $\nu = 4$, the exact high temperature ($T\to\infty$) limiting value of specific heat C is already known[5-8] and is given by $C/k_B = 3/4$ ($k_B \equiv$ Boltzmann constant); this result is trivially extended[9-12] to any value of ν ($C/k_B = 1/2 + 1/\nu$). In what concerns the leading correction to this limiting value it has been shown to be a $1/T^{(1+2/\nu)}$ term; however we shall see herein that the numerical coefficient provided by the approximate partition function ap-

pearing in Ref. [10] is asymptotically exact only in the neighbourhood of $\nu = 2$. For the low temperature region ($T \to 0$) a good approximation to the specific heat is available[5] for $\nu = 4$; we intend to present herein the exact $T \to 0$ asymptotic behavior for all values of ν. Also we numerically calculate, for typical values of ν, the specific heat for arbitrary values of T. All the specific heat analysis is presented in Section III.

II - ENERGY EIGENVALUES

The exact eigenvalues of Hamiltonian (1) were found[1] to be

$$E_n(\nu) = B(\nu)\ \frac{(-1)^n}{n!}\ \frac{d^n}{ds^n}\left[\frac{(2+s)^n}{s\left(1+\frac{2\nu}{\nu+2}\right)}\right]_{s\,=\,2} \qquad (n = 0,1,2\ldots) \qquad (2)$$

where

$$B(\nu) \equiv \hbar\omega(\nu)\left[\pi/2 \int_0^1 dq\ (1-q^\nu)^{1/2}\right]^{2\nu/(\nu+2)} \Gamma\left(1+\frac{2\nu}{\nu+2}\right) \qquad (3)$$

and

$$\omega(\nu) \equiv \frac{a}{m}\left[\hbar^{\frac{\nu-2}{\nu+2}}\right] \qquad (4)$$

Through straightforward mathematical processing we can rewrite expression (3) as follows:

$$B(\nu) = \hbar\omega(\nu)\left[\frac{\nu\Gamma(\frac{1}{2})\Gamma(\frac{1}{\nu}+\frac{3}{2})}{\Gamma(\frac{1}{\nu})}\right]^{\frac{2\nu}{\nu+2}}\Gamma\left(1+\frac{2\nu}{\nu+2}\right) \qquad (3')$$

The form (2) (together with (3') and (4)) is not a convenient one from the operational standpoint as, to obtain the n-th level, one needs to calculate all the preceding ones, and each of them envolves tedious derivative processing. Let us exhibit how these inconveniences can be overcome. Equation (2) can be rewritten as follows:

$$E_n(\lambda) = B(\lambda)\left\{\frac{(-1)^n}{n!}\sum_{\ell=0}^{n}\left[\binom{n}{\ell}2^{\ell}\frac{d^n}{ds^n}\left(s^{n-\ell-\lambda-1}\right)_{s=2}\right]\right\}$$

$$= \frac{B(\lambda)(-1)^n}{2^{1+\lambda}\,n!}\sum_{\ell=0}^{n}\binom{n}{\ell}\left\{\left[\prod_{p=1}^{n}(n-\ell-\lambda-p)\right]\left(1-\delta_{n,0}\right)+\delta_{n,0}\right\}$$

$$= \frac{B(\lambda)}{1+\lambda}\sum_{\ell=0}^{n}\frac{\Gamma(\lambda+\ell+1)}{\Gamma(\ell+1)\Gamma(n-\ell+1)\Gamma(\lambda+\ell+1-n)} \qquad (5)$$

where we have introduced a convenient variable $\lambda \equiv 2\nu/(\nu+2) \in (0,2)$ and where by $E_n(\lambda)$ and $B(\lambda)$ we strictly mean $E_n(\nu(\lambda))$ and $B(\nu(\lambda))$ (coherently with this convention we shall from now on use $\omega(\lambda)$ instead of $\omega(\nu(\lambda))$. Remark that

$$E_o(\lambda) = \frac{B(\lambda)}{2^{1+\lambda}} \qquad (6)$$

and that $E_n(\lambda)/E_o(\lambda)$ is a polynomial in λ of the n-th degree.

In the limit $\lambda \to 0$ the potential becomes an infinitely narrow well with depth $\frac{a}{2m}$, and an infinite degeneracy ap-

pears as all the energy levels are given by $E_n(0) = \frac{a}{2m}$ (in other words, we are in the limit of a free particle where all bound states disappear). For $\lambda = 1$ we recover the well known harmonic oscillator spectrum, i.e. $E_n(1) = \hbar\omega(1)(n+\frac{1}{2})$ $(\omega(1) \equiv a/m)$. In the limit $\lambda \to 2$ the potential becomes an infinite square well with width $2/\sqrt{a}$ and the spectrum is given by

$$E_n(2) = \frac{\pi^2\hbar\omega(2)}{8}(n^2+n+\frac{1}{2})$$

$$= \frac{\pi^2\hbar^2 a}{8m}(n^2+n+\frac{1}{2}) \qquad (7)$$

It is interesting to remark that the spectrum of the present "square well" is different from the standard one for which $E_n = \frac{\pi^2\hbar^2 a}{8m}(n+1)^2$ $(n = 0,1,2,\ldots)$. This is a non uniform convergence consequence: within the present procedure we take the limit $\nu \to \infty$ in the spectrum associated with a continuous potential (proportional to $|x|^\nu$) whereas within the standard procedure a discontinuous infinite square well is considered from the very beginning of the problem.

In Fig. 1 we present the evolutions, as a function of λ of the first six energy levels. For a pedagogical discussion of the wave functions corresponding to the $|x|^\nu$-type potential see Ref. [13].

Expression (5) is a quite convenient one for let us say spectroscopy-like purposes where particular levels have to be considered. But if we are interested in the knowledge of the whole spectrum (to perform thermal statistical averages for example) then recursive relations can be very useful. By using

the original expression (2) it is straightforward to establish (for $n = 0,1,2,\ldots$) that

$$\frac{E_n(\lambda+1)}{E_0(\lambda+1)} = \frac{n+1}{\lambda+1}\left[\frac{E_{n+1}(\lambda)}{E_0(\lambda)} + \frac{n-\lambda}{n+1}\frac{E_n(\lambda)}{E_0(\lambda)}\right] \tag{8}$$

and its inverse

$$\frac{E_{n+1}(\lambda)}{E_0(\lambda)} = \frac{n-\lambda}{\lambda+1}\left[\frac{n+1}{n-\lambda}\frac{E_n(\lambda+1)}{E_0(\lambda+1)} - \frac{E_{n+1}(\lambda+1)}{E_0(\lambda+1)}\right] \tag{9}$$

where we have used that $2E_0(\lambda+1)/E_0(\lambda) = B(\lambda+1)/B(\lambda)$. These relations show that it sufficient to discuss the interval $0 \leq \lambda \leq 1$ as the interval $1 < \lambda \leq 2$ can be trivially deduced from the former. By combining Eqs. (8) and (9) we finally obtain the following operationally useful recursive relation (for $n = 1,2,\ldots$)

$$E_{n+1}(\lambda) = \frac{1}{n+1}\left[(2\lambda+1)E_n(\lambda) + nE_{n-1}(\lambda)\right] \tag{10}$$

In Table I we compare, for typical values of n, the exact results for the energy eigenvalues associated with $\nu = 4,6,8$, to the approximate ones previously obtained[2-4]: we verify that their degree of confidence increases with n.

It is interesting for many purposes to know the asymptotic behaviour of $E_n(\lambda)$ for $n >> 1$. To exhibit this let us go back to expression (5) and present it as follows:

$$E_n(\lambda) = E_0(\lambda)\left[\frac{\Gamma(n+1+\lambda)}{\Gamma(1)\Gamma(\lambda+1)\Gamma(n+1)} + \frac{\Gamma(n+\lambda)}{\Gamma(2)\Gamma(\lambda)\Gamma(n)} + \frac{\Gamma(n-1+\lambda)}{\Gamma(3)\Gamma(\lambda-1)\Gamma(n-1)} + \cdots\right] \tag{11}$$

By using the fact that, in the limit $z \to \infty$, $\Gamma(z+\lambda)/\Gamma(z) \sim z^{\lambda}$ and also that $\sum_{\ell=0}^{\infty} \Gamma(\lambda+1)/[\Gamma(\ell+1)\Gamma(\lambda-\ell+1)] = 2^{\lambda}$, we can rewrite Eq. (11) as follows

$$E_n(\lambda) = E_o(\lambda) \frac{2^{\lambda} n^{\lambda}}{\Gamma(\lambda+1)} \left[1 + \frac{\lambda}{2n} + \frac{\lambda(\lambda^2-1)}{12n^2} + \ldots\right] \qquad (12)$$

or even

$$E_n(\lambda) = E_o(\lambda) \frac{2^{\lambda}(n+\frac{1}{2})^{\lambda}}{\Gamma(\lambda+1)} \left[1 + \frac{\lambda(\lambda-1)(2\lambda-1)}{24\left(n+\frac{1}{2}\right)^2} + \ldots\right] \qquad (13)$$

The leading term of the last expression coincides[14] with the well known WKB approximation, which is in fact exact for $\lambda = 0,1$; if we also take into account the second leading term, then expression (13) is exact for $\lambda = 2$ as well (as a matter of fact the error, for the most unfavorable values of λ, is less than 4% for $n = 1$, less than 2% for $n = 2$, and quickly decreases for increasing n).

III - SPECIFIC HEAT

The canonical partition function of the present anharmonic oscillator is given by

$$Z = \sum_{n=0}^{\infty} e^{-E_n(\lambda)/k_B T} \qquad (14)$$

whose knowledge immediately provides the specific heat through the relation

$$\frac{C}{k_B} = \frac{\partial}{\partial T}\left(T^2 \frac{\partial \ln Z}{\partial T}\right) = \frac{1}{(k_B T)^2} \left\langle \delta\rho^2 - \langle \delta\rho \rangle^2 \right\rangle \qquad (15)$$

where $\langle \ldots \rangle$ denotes mean thermal value.

A straightforward calculation leads, in the limit $T \to 0$, to

$$\frac{C}{k_B} \sim \left[\frac{2\lambda E_o(\lambda)}{k_B T}\right]^2 \exp\left[-\frac{2\lambda E_o(\lambda)}{k_B T}\right] \qquad (16)$$

We did not succeed in analytically performing the sum (14) for arbitrary values of λ and T. Therefore we turned onto a numerical treatment and the results are exhibited in Fig. 2 and Table II; for low values of λ and high values of T a great quantity of levels has to be considered in order to obtain satisfactory accuracy (for instance the knowledge of 3 significative figures in the discrepancy $\left[\frac{C_\lambda}{k_B} - 1\right](k_B T)^{2/\lambda}$ for $\lambda = 2/5$ and $k_B T/\hbar\omega(\lambda) \simeq 4$ demands to go up to levels corresponding to $n = 6 \times 10^5$).

Let us now discuss the high temperature region: it can be shown that, in the limit $T \to \infty$,

$$\frac{C}{k_B} \sim \frac{1}{\lambda}\left\{1 - R(\lambda)\left[\frac{\hbar\omega(\lambda)}{k_B T}\right]^{2/\lambda}\right\} \qquad (17)$$

where $R(\lambda)$ is a pure number whose analytic expression is still unknown. The present numerical results for C/k_B we mentioned in the previous paragraph enable us to calculate $R(\lambda)$: see Fig. 3 and Table III.

In what follows we shall deduce an anlytical approximation for $R(\lambda)$ which is extremely accurate for $\lambda \gtrsim 2/5$.

We substitute into Eq. (14), the exact spectrum by its asymptotic expression (12) and then, through the Euler-MacLaurin summation formula[15], we transform the sum into an integral, thus obtaining

$$Z \simeq \int_0^\infty dn \; e^{-\left\{\frac{E_o(\lambda)}{k_B T} \frac{2^\lambda n^\lambda}{\Gamma(\lambda+1)}\left[1 + \frac{\lambda}{2n} + \frac{\lambda(\lambda^2-1)}{12n^2}\right]\right\}} + \frac{1}{2}$$

$$= \int_0^\infty dn \; e^{-\frac{E_o(\lambda)}{k_B T} \frac{2^\lambda n^\lambda}{\Gamma(\lambda+1)}} \left\{ 1 - \frac{E_o(\lambda)}{k_B T} \frac{2^\lambda n^\lambda}{\Gamma(\lambda+1)} \left[\frac{\lambda}{2n} + \frac{\lambda(\lambda^2-1)}{12n^2}\right] \right.$$

$$\left. + \frac{1}{2}\left[\frac{E_o(\lambda)}{k_B T} \frac{2^\lambda n^\lambda}{\Gamma(\lambda+1)}\right]^2 \frac{\lambda^2}{4n^2} + \ldots \right\} + \frac{1}{2}$$

$$= \frac{\Gamma(1+\frac{1}{\lambda})}{2} \left[\frac{E_o(\lambda)}{\Gamma(\lambda+1) k_B T}\right]^{-\frac{1}{\lambda}} \left\{ 1 - \frac{(\lambda-1)(2\lambda-1)\Gamma(1-\frac{1}{\lambda})}{6\,\Gamma\left(\frac{1}{\lambda}+1\right)} \left[\frac{E_o(\lambda)}{\Gamma(\lambda+1) k_B T}\right]^{2/\lambda} \right.$$

$$\left. + \ldots \right\} \qquad (18)$$

This expression immediately leads, through Eq. (15), to Eq. (17) where $R(\lambda)$ is approximated as follows

$$R(\lambda) \simeq \frac{(\lambda-1)(2-\lambda)(2\lambda-1)\Gamma(1-\frac{1}{\lambda})}{12} \; \frac{\Gamma\left(\frac{1}{2}\right)^2 \Gamma(1/\lambda)}{2^{2/\lambda}\,\lambda^2\,\Gamma(\frac{1}{\lambda}+1/2)^2} \qquad (19)$$

Typical numerical results are presented in Fig. 3 and Table III. Eq. (19) represents a great improvement in the previously available work, namely that of Witschel[10] where the Wigner-Kirkwood semiclassical partition function formalism[16] is used to obtain a leading correction term with respect to

the classical partition function. Starting from the approximate partition function presented in Ref. [10] it is easy to deduce Eq. (17) with $R(\lambda)$ given by the following approximation:

$$R(\lambda) \simeq \frac{2\,\lambda\,\Gamma\left(\frac{5}{2}-\frac{1}{\lambda}\right)}{3\,\lambda\,2^{2/\lambda}(2-\lambda)\,\Gamma\left(\frac{1}{\lambda}-\frac{1}{2}\right)} \qquad (20)$$

For comparison purposes typical results calculated with this expression are presented in Fig. 3 and Table III.

IV - CONCLUSION

We have discussed the energy spectrum as well as the specific heat of a quantum single oscillator associated with a potential proportional to $|x|^{\nu}$ ($\nu > 0$). The exact eigenvalues available from Turschner recent work[1] have been further elaborated in order to achieve: (a) operationally convenient expression (namely Eq. (5)); (b) useful recursive relations (namely Eqs. (8)-(10)); (c) quite accurate asymptotic expressions in the limit $n \to \infty$ (namely Eqs. (12) and (13)).

In what concerns the specific heat we have obtained: (a) the exact asymptotic behaviour in the limit $T \to 0$ (namely Eq. (16)); (b) numerical results for typical values of ν and T (Fig. 2 and Table II); (c) the correct asymptotic form in the limit $T \to \infty$. To be more precise concerning the last point let us say that, for $T \to \infty$, C/k_B saturates at $(\frac{1}{2}+\frac{1}{\nu})$ and the leading correction is a $1/T^{1+\frac{2}{\nu}}$ term whose numerical coefficient has been both numerically calculated (Fig. 3 and Table

III) and analytically approximated (Eq. (19)).

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REFERENCES

1 - H. Turschner, J. Phys. A, 12, 451 (1979)

2 - F.T. Hioe and E.W. Montroll, J. Math. Phys. 16, 1945 (1975)

3 - K. Banerje, S.P. Bhatnagar, V. Choudry and S.S. Kanwal, proc. Roy. Soc. A 360, 575 (1978)

4 - F.T. Hioe, D. Macmillen and E.W. Montroll, J. Math. Phys, 17, 1320 (1976)

5 - M. Schwarz, Jr, J. Stat, Phys. 15, 255 (1976)

6 - C. Tsallis and J.W.F. Valle, Rev. Bras. Fis. 9, 759 (1979)

7 - R.A.T. Lima and C. Tsallis, Phys. Rev. B 21, 458 (1980)

8 - W. Witschel, Chem. Phys. Lett. 86, 558 (1982)

9 - L.R. da Silva and C. Tsallis, Rev. Bras. Fis. 9, 619 (1979)

10 - W. Witschel, Chem. Phys. Lett. 71 , 131 (1980)

11 - W. Witschel, Z. Naturforsch 36a, 481. (1981)

12 - C. Tsallis and L.R. da Silva, Phys. Rev. A 25(1982)

13 - P.M. Oliveira and A.M. Mariz, to be published.

14 - K. Banerjee, Proc. Roy. Soc. A 364, 265 (1978)

15 - G.A. Korn and T.M. Korn, Mathematical Handbook for scientists and engineers, 2th ed.(MC Graw-Hill Book Company, 1968) p. 125

16 - L.D. Landau and E.M. Lifshitz, Statistical Physical, 1th ed. (Pergamon Press, London , 1958)

CAPTION FOR TABLES AND FIGURES

Table I - Selected levels of the approximate and exact energy spectra for typical values of ν((a) ν=4; (b) ν=6; (c) ν=8).

Table II - Specific heat (exact) for selected values of the temperature T and ν.

Table III - Exact and approximate values of the high-temperature coefficient $R(\lambda)$ (see eq. (17)) for selected values of $\lambda = 2\nu/(\nu+2)$.

Fig. 1 - Fundamental and excited levels of the energy spectrum (exact) as a function of $\lambda \equiv 2\nu/(\nu+2)$

Fig. 2 - Thermal dependence of the exact specific heat corresponding to selected values of ν.

Fig. 3 - The high-temperature coefficient $R(\lambda)$ (see eq. (17)) as function of $\lambda \equiv 2\nu/(\nu+2)$. Continuous: exact (numerical), it attains its maximum value in the neighbourhood of $\lambda = 4/3$; dot-dashed: First analytic proposal (eq. (19), it diverges at $\lambda = 1/3$; dashed: Second analytic proposal (eq. (20) deduced by us from [10]), it diverges at $\lambda = 2/5$.

TABLE I

n	$E_n(\nu=4)/\hbar\omega(\nu=4)$ (a)		
	HIOE(1975) *	BANERJEE(1978)	EXACT
0	0.530181	0.530181	0.516229...
1	1.899837	1.899837	1.892838...
10	25.121335	25.128127	25.127242...
50	203.934508	203.937182	203.936825...
100	510.493269	510.494996	510.494769...
1000	10932.630648	10932.631059	10932.631010...
10000	235395.146537	235395.147214	235395.147202...

n	$E_n(\nu=6)/\hbar\omega(\nu=6)$ (b)	
	HIOE(1876)	EXACT
0	0.572404	0.532288...
1	2.169303	2.129151...
2	4.536544	4.524447...
3	7.467589	7.452030...
4	10.857066	10.845365...
5	14.649761	14.637916...

n	$E_n(\nu=8)/\hbar\omega(\nu=8)$ (c)	
	HIOE(1976)	EXACT
0	0.612911	0.544641...
1	2.377909	2.287492...
2	5.122494	5.076054...
3	8.671641	8.631471...
4	12.905042	12.870085...
5	17.749655	17.716048...

* These values were calculated by using Eqs.(IV.15) and (IV.16) of Ref. [2].

TABLE II

C/k_B / $k_BT/\hbar\omega(\nu)$	$\nu = 1/2$	$\nu = 1$	$\nu = 2$ *	$\nu = 4$	$\nu \to \infty$
0.2	1.150874	0.505332	0.170742	0.048489	0.000669
0.4	2.309754	1.133296	0.608890	0.376005	0.079332
0.6	2.451448	1.345011	0.797441	0.558937	0.268633
0.8	2.483854	1.423335	0.879366	0.633695	0.405651
1.0	2.493504	1.457285	0.920674	0.669246	0.467745
1.2	2.497000	1.474010	0.944085	0.689473	0.490114
1.4	2.498465	1.483099	0.958546	0.702307	0.497182
1.6	2.499150	1.488428	0.968074	0.711103	0.499237
1.8	2.499499	1.491746	0.974672	0.717465	0.499801
2.0	2.499689	1.493914	0.979425	0.722251	0.499950

*The analytic expression corresponding to $\nu = 2$ is given by[16]

$$\frac{C}{k_B} = \frac{\theta^2 \exp(\theta)}{\left[\exp(\theta)-1\right]^2} \qquad \left(\theta \equiv \frac{\hbar\omega(\upsilon=2)}{k_B T}\right)$$

TABLE III

λ	$R(\lambda)$		
	Exact	Eq.(19)	Eq. (20)
0.4	0.006...	0.008	∞
2/3	0.034...	0.034	0.042
0.8	0.055...	0.055	0.058
1.0	1/12	0.833	0.833
1.2	0.101...	0.101	0.106
4/3	0.104...	0.104	0.119
1.4	0.105...	0.103	0.126
1.6	0.087...	0.087	0.142
1.8	0.053...	0.053	0.155
2.0	0	0	0.167

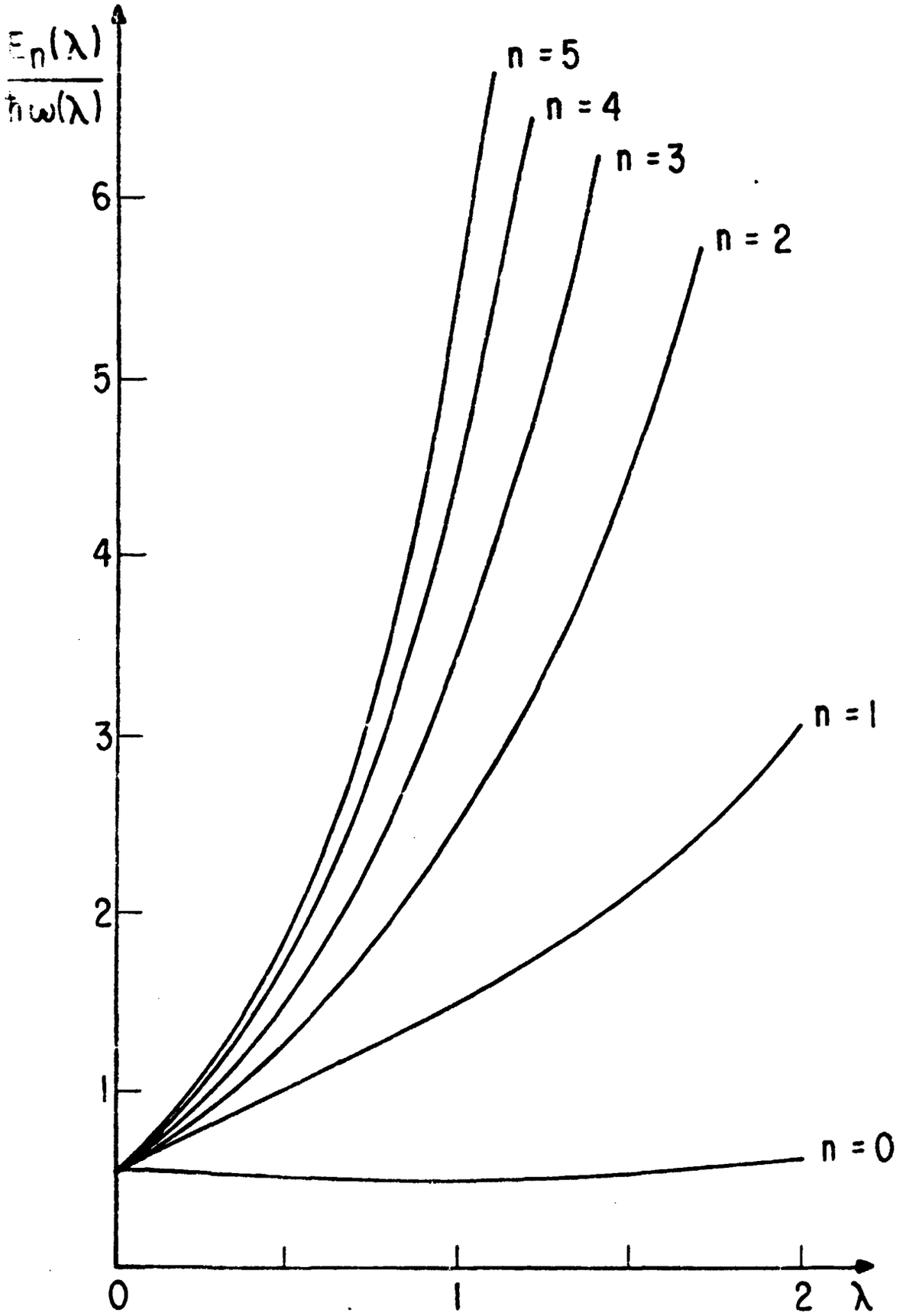

FIG.1

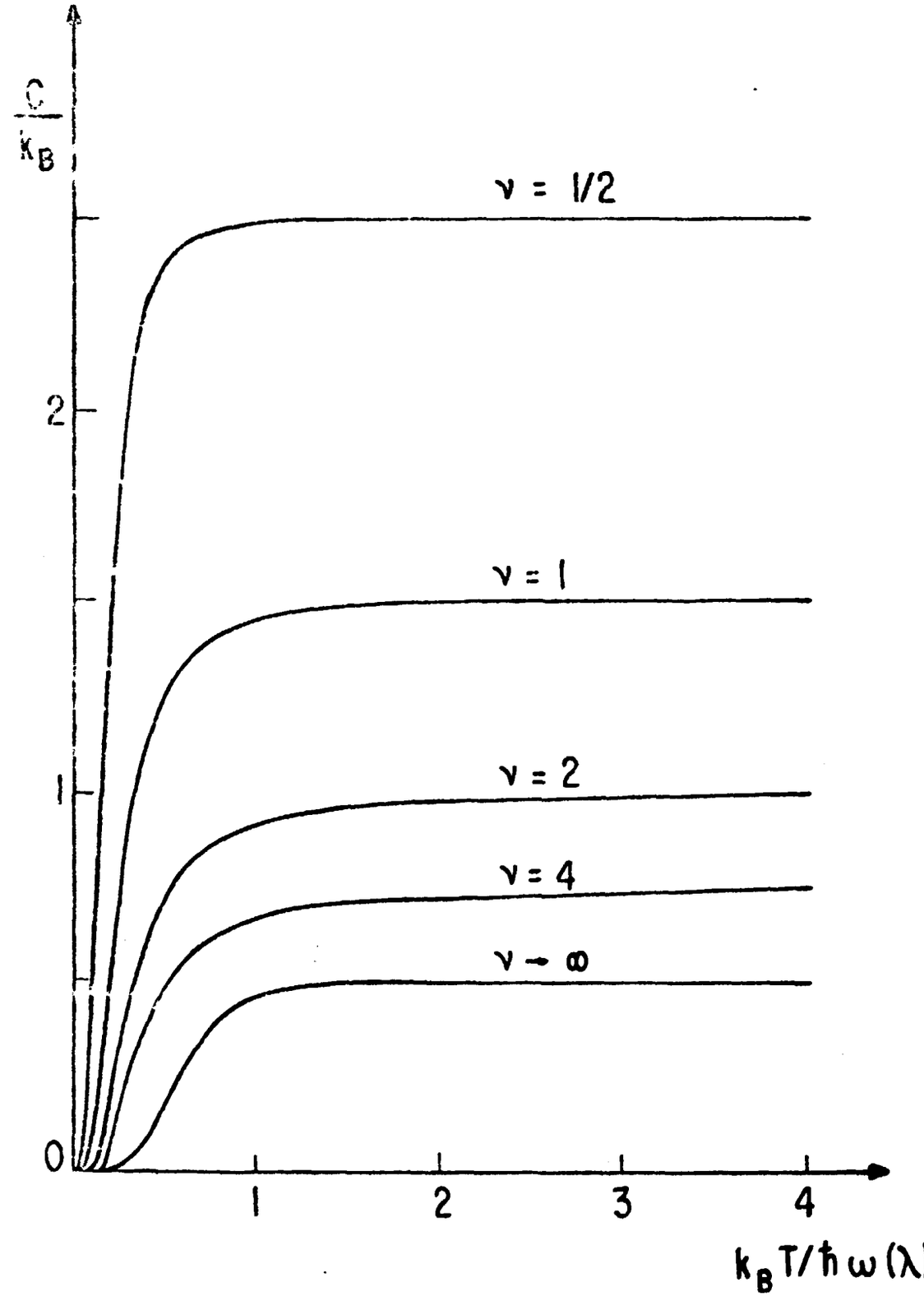

FIG. 2

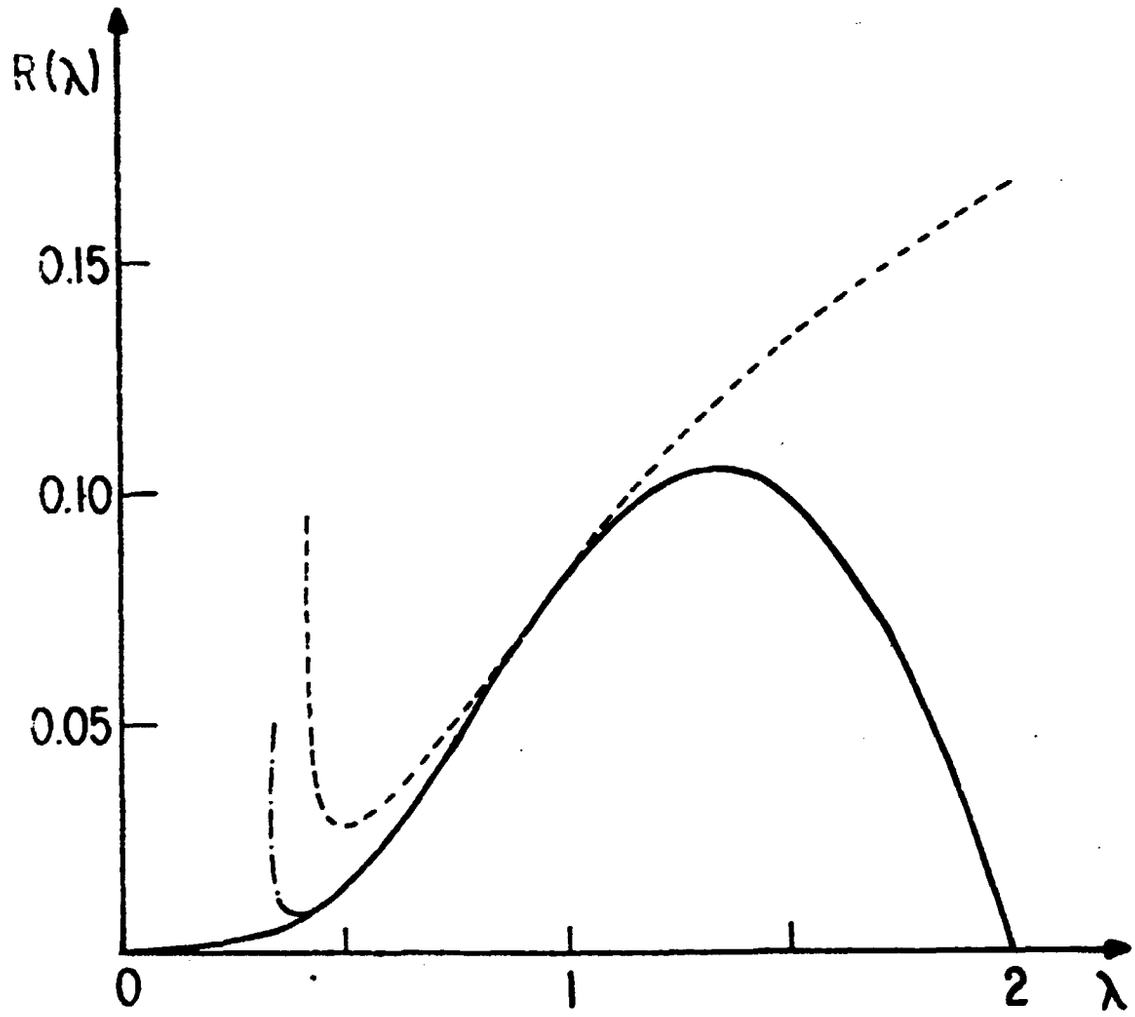

FIG.3

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