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Specific Heat of the Anisotropic Rigid Rotator within Generalized Statistics

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Abstract

Within a recently generalized statistical mechanics, we have calculated the specific heat of a classical and quantum anisotropic rigid rotator. In addition to this, we extend Hilhorst's formula to the grand-canonical ensemble.

Key-words: Generalized Statistics; Rigid Rotator; Specific Heat; Nonextensive Systems.

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1.- Introduction

There are few quantum systems whose energy spectrum is exactly known. Among them we have the anisotropic (oblate and prolate) rigid rotator. Its specific heat within standard Boltzmann-Gibbs statistics was numerically studied in [1]. A generalization of the Boltzmann-Gibbs statistics has been recently proposed for nonextensive systems [2-4], and its connection with thermodynamics is now established [5]. This generalization relies on an entropy $S_q \equiv k(1 - \sum_i p_i^q)/(q-1)$, ($q \in \Re$; k is a conventional positive constant) which recovers, in the limit $q \to 1$, the standard one $-k_B \sum_i p_i \ln p_i$. Various properties of the generalized entropy have been proved, such as positivity, equiprobability, expansibility, concavity and H-theorem [6-8]. This generalized statistics has been shown to satisfy appropriate forms of the Ehrenfest theorem [9], von Neumann equation [10], Bogolyubov inequality [11], Langevin and Fokker-Planck equations [12], Callen's identity (used to calculate the critical temperature of the Ising ferromagnet) [13], Fluctuation-dissipation and Onsager reciprocity theorems [14] and quantum statistics [15]. This generalization was applied to calculate the thermal dependence of the specific heat associated with the $d = 1$ Ising ferromagnet [16], a confined free particle (square well) [17], two-level system and harmonic oscillator [18].

Finally, this formalism has already received physical and mathematical applications. Among them we have the following situations: (i) Plastino and Plastino [19], for the polytropic model for self-gravitating stellar systems, and Aly [19], on more general grounds, have shown that, if q sufficiently differs from unity, it is possible to have *simultaneously finite* mass, energy and entropy, thus solving a classical difficulty of Boltzmann-Gibbs statistical mechanics; (ii) Alemany and Zanette [20] have shown that, by appropriately choosing q, it is possible to variationally obtain (with simple auxiliary conditions) Lévy distributions, even when the $q = 1$ formalism fails, i.e., when the displacement second moment *diverges* (which is indeed the case for CTAB micelles in salted water [21], heartbeat histograms [22], among others); (iii) Landsberg [23] considers the possibility of having applications in self-organizing biological systems; (iv) the well known Student t-distribution and r-distribution can be variationally obtained from an entropic principle [24]; (v) The Simulated Annealing optimization algorithms can be generalized [25] in such a way as to become much quicker.

In the present paper, we will study, for arbitrary q, the thermal behavior of the specific heat of a large class of anisotropic rigid rotators . In Section 2, the quantum results are presented for typical values of the momenta of inertia. In Section 3, the classical case is studied, and the quantum and classical behaviors are compared. In both Sections, it is verified that the traditional results of the Boltzmann-Gibbs statistics are recovered as the $q = 1$ particular case of the generalized statistics. In Section 4 we extend Hilhorst formula to the grand canonical ensemble.

2.- Quantum Case

We address here the generalized specific heat C_q of the most general anisotropic rigid rotator with axial symmetry (oblate, spherical, prolate). The spectrum of energy of this rotator is given [26] by

$$E_{l,m} = \frac{\hbar^2}{2I_{xy}} \left(l(l+1) + (\frac{I_{xy}}{I_z} - 1)m^2 + \epsilon_o \right), \qquad (1)$$

where $l = 0, 1, 2, 3, ...$ represents the eigenvalues of the angular momentum operator, $m = -l, -l+1, ..., l$ its possible projections on the intrinsic rotation axis of the rotator, each state has a degeneracy $(2l+1)$, $I_x = I_y \equiv I_{xy}$ and I_z are the associated momenta of inertia, and ϵ_o is an arbitrary additive constant. The generalized partition function can be written

$$Z_q(\beta) = \sum_{l=0}^{\infty}(2l+1) \sum_{m=-l}^{l} [1 - \beta(1-q)E_{l,m}]^{\frac{1}{1-q}} ,$$

where $\beta \equiv 1/kT$, T being the temperature. Now, if we define Z_q in terms of the reduced quantities $b \equiv \hbar^2\beta/2I_{xy}$ and $\epsilon_{l,m} \equiv 2I_{xy}E_{l,m}/\hbar^2$, we obtain

$$Z_q(b) = \sum_{l=0}^{\infty}(2l+1) \sum_{m=-l}^{l} [1 - b(1-q)\epsilon_{l,m}]^{\frac{1}{1-q}} . \qquad (2)$$

Let us also define

$$V_q(b) \equiv \sum_{l=0}^{\infty}(2l+1) \sum_{m=-l}^{l} [1 - b(1-q)\epsilon_{l,m}]^{\frac{q}{1-q}-1} \epsilon_{l,m}^2, \qquad (3)$$

and

$$W_q(b) \equiv \sum_{l=0}^{\infty}(2l+1) \sum_{m=-l}^{l} [1 - b(1-q)\epsilon_{l,m}]^{\frac{q}{1-q}} \epsilon_{l,m}. \qquad (4)$$

The generalized internal energy U_q is given [5] by $U_q = -\frac{\partial}{\partial\beta}\frac{Z_q^{1-q}(\beta)-1}{1-q}$. For convenience, we introduce the reduced internal energy as $u_q \equiv 2I_{xy}U_q/\hbar^2$ which is given by

$$u_q(b) = \frac{W_q(b)}{[Z_q(b)]^q}. \qquad (5)$$

Consequently, the specific heat $C_q = \partial U_q/\partial T$ is given by

$$\frac{C_q(t)}{k} = \frac{q}{t^2} \left\{ \frac{V_q(1/t)}{[Z_q(1/t)]^q} - \frac{[W_q(1/t)]^2}{[Z_q(1/t)]^{q+1}} \right\}, \qquad (6)$$

where we have introduced the reduced temperature $t \equiv 1/b$. This equation enables the numerical calculation of $C_q(t)$. In [1], it was solved the case of the anisotropic rigid rotator within the Boltzmann-Gibbs statistics (q=1). Those results are exactly recovered in this new formalism when $q \to 1$ and for all values of ϵ_o (see Fig.1).

Before going on, let us make a brief historical digression and mention that we can see in Fig.1 the solution of the "*paradox*" that deeply disturbed J. W. Gibbs. Indeed, in the introduction of his celebrated 1901 "*Elementary Principles in Statistical Mechanics, Developed with Especial Reference to the Rational Foundation of Thermodynamics*" he writes "*It is well known that while theory would assign to the* [diatomic] *gas six degrees of freedom per molecule, in our experiments on specific heat we cannot account for more than five. Certanly, one is building on an insecure foundation, who rests his work on hypothesis concerning the constitution of matter. Difficulties of this kind have deterred the author from attempting to explain the mysteries of nature, and have forced him to be contented with the more modest aim of deducing some of the more obvious propositions relating to the statistical branch of mechanics.*" The six degrees of freedom which Gibbs refer to are, of course, three translational (which are trivial) and three rotational (responsible for the " *paradox*"). Fig.1 clearly exhibits what happens with the rotational ones. If $I_{xy}/I_z >> 1$, the specific heat behaves like a *two*-degree system until very high temperatures (experimentally inaccessible in the standard situations) are achieved, above which the *third* degree of freedom becomes thermally active. As we shall exhibit later on, the same type of nonuniform convergence remains for $q \neq 1$.

Let us now go back to our discussion. For $q \neq 1$ and $\epsilon_o = 0$ the situation is well illustrated through the study of three typical cases, namely $I_{xy}/I_z = 1/2$ (extremely prolate), $I_{xy}/I_z = 1$ (spherical) and $I_{xy}/I_z \to \infty$ (extremely oblate) :

(*i*) For $q > 1$, $C_q \geq 0$ and the high-temperature asymptotic behavior is modified; indeed, $\lim_{t\to\infty} C_q = 0$, in constrat with the $q = 1$ statistics ($C_1/k \to 3/2$ for all finite ratios I_{xy}/I_z). Our numerical results suggest that for $q \geq 5/3$, $C_q(t) = 0$ $\forall\ t > 0$. For $1 < q < 5/3$, both $C_q(t)$ and $dC_q(t)/dt$ are continuous (the $q = 4/3$ case is depicted Fig.2*a*).

(*ii*) For $0 < q < 1$, $C_q \geq 0$ and the high-temperature asymptotic behavior is once again modified $\lim_{t\to\infty} C_q = \infty$. We can distinguish three cases. Again, our numerical results suggest that for $2/3 < q < 1$, $C_q(t)$ function is continuous, differentiable and presents an infinite number of extrema (the $q = 5/6$ case is despicted in Fig.2*b*); for $1/2 < q < 2/3$, $C_q(t)$ is continuous, but $dC_q(t)/dt$ presents discontinuities at the values $t_{l,m} = (1-q)\epsilon_{l,m}$ (the $q = 7/12$ case is despicted in Fig.2*c*); finally, for $0 < q < 1/2$, $C_q(t)$ itself presents discontinuites at the values $t_{l,m} = (1-q)\epsilon_{l,m}$ (the $q = 1/3$ case is shown in Fig.2*d*). In all these cases, the $0 \leq t \leq (1-q)[2-(1-I_{xy}/I_z)\Theta(1-I_{xy}/I_z)]$ region (where $\Theta(x)$ is the step function), is *thermally frozen* (*i.e.,* only the ground state is polpulated).

(*iii*) For $q < 0$, $C_q(t) \leq 0\ \forall\ t > 0$ and presents discontinuities at the values $t_{l,m} = (1-q)\epsilon_{l,m}$.

The presence of a nonvanishing zero-point ($\epsilon_o \neq 0$) is, of course, irrelevant when $q = 1$. This is not so when $q \neq 1$. We remark that:

(*i*) For $1 < q < 5/3$ and $\epsilon_o > 0$, $C_q(t)$ is continuous and positive everywhere, excepting at $t = 0$, where it vanishes. But if $\epsilon_o < 0$, the $0 \leq t \leq (1-q)\epsilon_o$ is a thermally frozen region (see Appendix A.1) hence $C_q(t)$ vanishes; $C_q(t)$ is positive and continuous for $t > (1-q)\epsilon_o$. (The case $q = 4/3$ and $I_{xy}/I_z = 1$ is depicted in Fig.3*a* for ϵ_o = -1, 0, 1).

(*ii*) For $0 < q < 1$ and $\epsilon_o > 0$, the region $0 \le t \le (1-q)\epsilon_o$ is *thermally forbidden* (physically inaccessible); the region $(1-q)\epsilon_o \le t \le (1-q)[2+\epsilon_o-(1-I_{xy}/I_z)\Theta(1-I_{xy}/I_z)]$ is thermally frozen. When $-2 < \epsilon_o < 0$, the region $0 < t < (1-q)[2-|\epsilon_o|-(1-I_{xy}/I_z)\Theta(1-I_{xy}/I_z)]$ is thermally frozen, when $\epsilon_o < -2$, C_q is positive everywhere. All cases present the discontinuities before described for C_q and dC_q/dt respectively. (The $q = 2/3$ and $I_{xy}/I_z = 1$ case is shown in the Fig.3*b* for ϵ_o = -3, -1, 0, 2).

3.- Classical Case

For $q > 1$, the classical expresion for the Eq.(2) can be obtained by using the well known $q = 1$ partition function into Hilhorst formula [3] and the well known $q = 1$ specific heat. So the $\epsilon_o = 0$ generalized classical partition function is given by

$$Z_q^{class}(t) = \frac{\pi^{1/2}}{\sqrt{I_{xy}/I_z}} \frac{\Gamma(\frac{1}{q-1}-\frac{3}{2})}{(q-1)^{3/2}\Gamma(\frac{1}{q-1})} t^{3/2}, \tag{7}$$

The classical internal energy is analogously obtained (see Appendix A.2) from Eq.(5) and is given by

$$u_q^{class}(t) = \frac{3}{2}\left(\frac{\pi^{1/2}}{\sqrt{I_{xy}/I_z}} \frac{\Gamma(\frac{1}{q-1}-\frac{3}{2})}{(q-1)^{3/2}\Gamma(\frac{1}{q-1})}\right)^{1-q} t^{1+\frac{3}{2}(1-q)}, \tag{8}$$

hence, for $q > 1$ and $\epsilon_o = 0$, we have

$$\frac{C_q^{class}(t)}{k} = \frac{3}{2}\left(1+\frac{3}{2}(1-q)\right)\left(\frac{\pi^{1/2}}{\sqrt{I_{xy}/I_z}} \frac{\Gamma(\frac{1}{q-1}-\frac{3}{2})}{(q-1)^{3/2}\Gamma(\frac{1}{q-1})}\right)^{1-q} t^{\frac{3}{2}(1-q)}. \tag{9}$$

For $1 < q < 5/3$ the specific heat has nonnegative value, diverges in the $t \to 0$ limit and vanishes in the $t \to \infty$ one; for $q \to 1$ we recover the well known result $C_1^{class}/k = 3/2$, $\forall t$.

For $q < 1$ the classical expresion is obtained by replacing, in the Eqs.(2), (5) and (6), the sums by integrals. We obtain, for $\epsilon_o = 0$,

$$Z_q^{class}(t) = \frac{\pi^{1/2}}{\sqrt{I_{xy}/I_z}} \frac{(1+\frac{3}{2}(1-q))^{-1}\Gamma(\frac{1}{1-q})}{(1-q)^{3/2}\Gamma(\frac{1}{1-q}+\frac{3}{2})} t^{3/2} \tag{10}$$

for the partition function,

$$u_q^{class}(t) = \frac{3}{2}\left(\frac{\pi^{1/2}}{\sqrt{I_{xy}/I_z}} \frac{(1+\frac{3}{2}(1-q))^{-1}\Gamma(\frac{1}{1-q})}{(1-q)^{3/2}\Gamma(\frac{1}{1-q}+\frac{3}{2})}\right)^{1-q} t^{1+\frac{3}{2}(1-q)} \tag{11}$$

for the internal energy and

$$\frac{C_q^{class}(t)}{k} = \frac{3}{2}\left(1+\frac{3}{2}(1-q)\right)\left(\frac{\pi^{1/2}}{\sqrt{I_{xy}/I_z}}\frac{(1+\frac{3}{2}(1-q))^{-1}\Gamma(\frac{1}{1-q})}{(1-q)^{3/2}\Gamma(\frac{1}{1-q}+\frac{3}{2})}\right)^{1-q} t^{\frac{3}{2}(1-q)} \qquad (12)$$

for the specific heat. For $0<q<1$ the specific heat has nonnegative values, vanishes in the $t\to 0$ limit and diverges in the $t\to\infty$ one; for $q\to 1$ we recover once more the result $C_1^{class}/k = 3/2$, $\forall t$.

The classical and quantum specific heats asymptotically coincide for $t >> 1$, $\forall\ \epsilon_o$, $\forall I_{xy}/I_z$, and for q above a critical value (which seems to be $q=1/2$; for $q\in(-\infty,1/2)$ the situation is more complex; in particular, for $q<0$, $C_q\le 0$ whereas $C_q^{class}\ge 0$). This is illustrated in Fig.4 for typical situations. Also, in what concerns the $I_{xy}/I_z\to\infty$ limit, we exhibit in Fig.5, for both $q>1$ and $q<1$ the same type of nonuniform convergence which occurs within Boltzmann-Gibbs statistics ($q=1$). Indeed, quantum and classical specific heats merge into a single curve above a temperature which increases with increasing ratio I_{xy}/I_z, and finally diverges in the $I_{xy}/I_z\to\infty$, thus yielding a degree of freedom which remains frozen for ever.

4.- Extension of the Hilhorst Formula to the Grand Canonical Ensemble

The equilibrium distribution for the grand-canonical ensemble is given by

$$p_j^{(N)} = \left[1-\beta(1-q)(E_j^{(N)}-\mu N)\right]^{\frac{1}{1-q}} / \Xi_q(\beta,\mu), \qquad (13)$$

where the number of particles $N=0,1,2...$, and $E_j^{(N)}$ represents the N-particle energy spectrum (characterized by the quantum number or set of quantum numbers j).
The generalized grand partition function is given by

$$\Xi_q(\beta,\mu) = \sum_{N=0}^{\infty}\sum_j \left[1-\beta(1-q)(E_j^{(N)}-\mu N)\right]^{\frac{1}{1-q}} . \qquad (14)$$

The associated constraints in the entropy optimization problem are as follows:

$$\sum_{N=0}^{\infty}\sum_j p_j^{(N)} = 1 \ , \qquad (15)$$

$$\sum_{N=0}^{\infty}\sum_j \left(p_j^{(N)}\right)^q E_j^{(N)} = U_q \ , \qquad (16)$$

and

$$\sum_{N=0}^{\infty} N \sum_j \left(p_j^{(N)}\right)^q = N_q \ . \qquad (17)$$

It is convenient to remark that in general

$$p^{(N)} \equiv \left[\sum_j \left(p_j^{(N)}\right)^q\right]^{1/q} \neq \sum_j p_j^{(N)} \equiv p_N \tag{18}$$

where p_N is the probability of having N particles (no matters the energy value) and $p^{(N)}$ is the quantity wich enables the re-writting of Eq.(17) as $\sum_{N=0}^{\infty} N(p^{(N)})^q = N_q$; unless $q = 1$, p_N generically differs from $p^{(N)}$ (for instance, $\sum_{N=o}^{\infty} p_N = 1$ always, whereas in general $\sum_{N=0}^{\infty} p^{(N)} \neq 1$).
From the standard representation of the Gamma function we have

$$\eta^{-\nu} = \frac{1}{\Gamma(\nu)} \int_0^{\infty} dx x^{\nu-1} e^{-\eta x}. \tag{19}$$

By using this in the generalized grand partition function (14) with the identifications $\nu = 1/(q-1)$ and $\eta = 1 + \beta(q-1)(E_j^{(N)} - \mu N)$, we obtain

$$\Xi_q(\beta,\mu) = \frac{1}{\Gamma(\frac{1}{q-1})} \sum_{N=0}^{\infty} \sum_j \int_0^{\infty} dx x^{\frac{1}{q-1}-1} \exp\Big(-[1 + \beta(q-1)(E_j^{(N)} - \mu N)]x\Big). \tag{20}$$

Whenever

$$\sum_{N=0}^{\infty} \sum_j \int_0^{\infty} dx = \int_0^{\infty} dx \sum_{N=0}^{\infty} \sum_j \quad , \tag{21}$$

Eq.(20) becomes

$$\Xi_q(\beta,\mu) = \frac{1}{\Gamma(\frac{1}{q-1})} \int_0^{\infty} dx x^{\frac{1}{q-1}-1} e^{-x} \sum_{N=0}^{\infty} \sum_j \exp\Big(-\beta(q-1)(E_j^{(N)} - \mu N)x\Big). \tag{22}$$

If we consider now $\alpha = \beta(q-1)x$, we obtain finally

$$\Xi_q(\beta,\mu) = \frac{1}{\Gamma(\frac{1}{q-1})[\beta(q-1)]^{\frac{1}{q-1}}} \int_0^{\infty} d\alpha \alpha^{\frac{1}{q-1}-1} e^{-\frac{\alpha}{\beta(q-1)}} \Xi_1(\alpha,\mu) \quad (q > 1)\ , \tag{23}$$

which extends to the grand-canonical ensemble the Hilhorst formula. The analogous expresion for the internal energy is given (see Appendix A.2) by

$$U_q(\beta,\mu) = \frac{1}{[\Xi_q(\beta,\mu)]^q \Gamma(\frac{q}{q-1})[\beta(q-1)]^{\frac{q}{q-1}}} \int_0^{\infty} d\alpha \alpha^{\frac{q}{q-1}-1} e^{-\frac{\alpha}{\beta(q-1)}} \quad \Xi_1(\alpha,\mu) U_1(\alpha,\mu) \qquad (q > 1) \tag{24}$$

5.- Conclusion

In any good Quantum Mechanics textbook we find *five* simple systems, namely, the $d = 1$ confined free particle (square well), the $d = 1$ harmonic oscillator, the spin 1/2 (or two level system), the Hydrogen atom and rigid rotator. It is in principle desirable to have the $q \neq 1$ basic statistical mechanics (e. g., specific heat) of them all. The free particle has been discussed in [17], the harmonic oscillator in [18], the two-level system in [2, 4, 18], and the Hydrogen atom in [27] (notice, by the way, that its $q = 1$ statistics cannot be calculated because of the long range interaction; e.g., the Boltzmann-Gibbs partition function *diverges*). In the present paper, by discussing the rigid rotator, we essentially close the study of the above mentioned set of elementary problems. Our main results for the rigid rotator are:

(i) For *all* values of the index q, the momenta ratio I_{xy}/I_z (from extremely prolate, $I_{xy}/I_z = 1/2$, to extremely oblate, $I_{xy}/I_z \to \infty$, passing through the spherical symmetry, $I_{xy}/I_z = 1$) and the aditive constant ϵ_o , the quantum specific heat C_q asymptotically coincides with the classical one C_q^{class}, which is proportional to $T^{\frac{3}{2}(1-q)}$.

(ii) For $q \geq 5/3$, C_q (possibly) vanishes for all temperatures; for $1 < q < 5/3$, C_q is continuous and differentiable almost everywhere (in *all* the thermally active region),vanishes at $T = 0$, and presents a frozen region ($C_q = 0$) if $\epsilon_o < 0$ (otherwise, i.e., for $\epsilon_o \geq 0$, the entire $T \neq 0$ region is thermally active); for $q \to 1 \pm 0$, we recover the Boltzmann-Gibbs results [1], $\forall \epsilon_o$; for $2/3 < q < 1$, C_q is continuous and differentiable in all the active region, it presents an infinite number of extrema, and it presents (if $\epsilon_o \geq 0$) both forbidden and frozen regions; for $1/2 \leq q \leq 2/3$, C_q is continuous but dC_q/dT presents an infinite number of discontinuities; for $0 < q < 1/2$, C_q itself presents an infinite number of divergences; $\lim_{q\to+0} C_q \neq \lim_{q\to-0}$; for $q < 0$, C_q is nonpositive, and presents an infinite number of divergences.

(iii) The peculiar 2-to-3-degrees-of-freedom crossover which occurs in the $I_{xy}/I_z \to \infty$ limit (and which worried Gibbs!) remains, for $q \neq 1$, essentially the same as within Boltzmann-Gibbs statistics ($q = 1$).

(iv) By following, for $q > 1$, along the lines of Hilhorst formula for the partition function Z_q, we obtain the analogous expression for the internal energy (in the canonical ensemble) as well as for both partition function and internal energy in the grand-canonical ensemble.

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Appendix A.1

If $q > 1$ and $\epsilon_o < 0$ it is convenient to stress that the canonical distribution will be given, for $t > (q-1)|\epsilon_o|$, by

$$p_{l,m} = (1 - b(1-q)\epsilon_{l,m})^{\frac{1}{1-q}} / Z_q(b), \tag{25}$$

but, if $t \leq (q-1)|\epsilon_o|$, then

$$p_{l,m} = \begin{cases} 1, & \text{if } l = m = 0; \\ 0, & \text{otherwise,} \end{cases} \tag{26}$$

Consequently, if $0 \leq t \leq (q-1)|\epsilon_o|$

$$u_q = \epsilon_0 \tag{27}$$

and

$$C_q = 0 \tag{28}$$

Appendix A.2

The Hilhorst formula is

$$Z_q(\beta) = \frac{1}{\Gamma(\frac{1}{q-1})[\beta(q-1)]^{\frac{1}{q-1}}} \int_0^\infty d\alpha \alpha^{\frac{1}{q-1}-1} e^{-\frac{\alpha}{\beta(q-1)}} Z_1(\alpha) \quad (q > 1) \tag{1}$$

If in the general expression for the internal energy

$$U_q(\beta) = \sum_j (1 - \beta(1-q)E_j)^{\frac{q}{1-q}} / [Z_q(\beta)]^q, \tag{2}$$

we identify $\nu = q/(q-1)$ and $\eta = 1 + \beta(q-1)E_j$ in the definition of the Gamma function (see Eq.(19)), we obtain

$$U_q(\beta) = \frac{1}{[Z_q(\beta)]^q \Gamma(\frac{q}{q-1})} \sum_j \int_0^\infty dx x^{\frac{q}{q-1}-1} e^{-(1+\beta(q-1)E_j)x} E_j. \tag{3}$$

Whenever

$$\sum_j \int_0^\infty dx = \int_0^\infty dx \sum_j \quad , \tag{4}$$

this equation becomes

$$U_q(\beta) = \frac{1}{[Z_q(\beta)]^q \Gamma(\frac{q}{q-1})} \int_0^\infty dx x^{\frac{q}{q-1}-1} e^{-x} \sum_j e^{-\beta(q-1)E_j x} E_j \quad . \tag{5}$$

If we consider now $\alpha = \beta(q-1)x$, we obtain finally

$$U_q(\beta) = \frac{1}{[Z_q(\beta)]^q \Gamma(\frac{q}{q-1})[\beta(q-1)]^{\frac{q}{q-1}}} \int_0^\infty d\alpha \alpha^{\frac{q}{q-1}-1} e^{-\frac{\alpha}{\beta(q-1)}} Z_1(\alpha) U_1(\alpha) \quad (q > 1) \tag{6}$$

which extends to the internal energy the type of relationship Hilhorst established for the partition function. Naturally, the treatment we have applied here to the Hamiltonian can be applied to any other observable.

Figures

Fig.1 Specific heat C_1/k as a function of the reduced temperature $t = 2I_{xy}kT/\hbar^2$ for typical values of I_{xy}/I_z.

Fig.2 Specific heat C_q/k as a function of the reduced temperature $t = 2I_{xy}kT/\hbar^2$ for $\epsilon_o = 0$ and typical values of I_{xy}/I_z and for different values of q, (a) $q = 4/3$ (b) $q = 5/6$, (c) $q = 7/12$ and (d) $q = 1/3$.

Fig.3 Specific heat C_q/k for typical values of ϵ_o, $I_{xy}/I_z = 1$ and (a) $q = 4/3$, (b) $q = 0.8$.

Fig.4 Comparison, for q=1.2, 0.8 and $\epsilon_o = 0$, of the classical (dashed lines) and quantum (full lines) specific heats for typical values of I_{xy}/I_z.

Fig.5 Classical (dashed lines) and quantum (full lines) specific heats for $\epsilon_o = 0$ and $I_{xy}/I_z >> 1$: (a) $q = 1.2$; (b) $q = 0.8$.

Fig.1

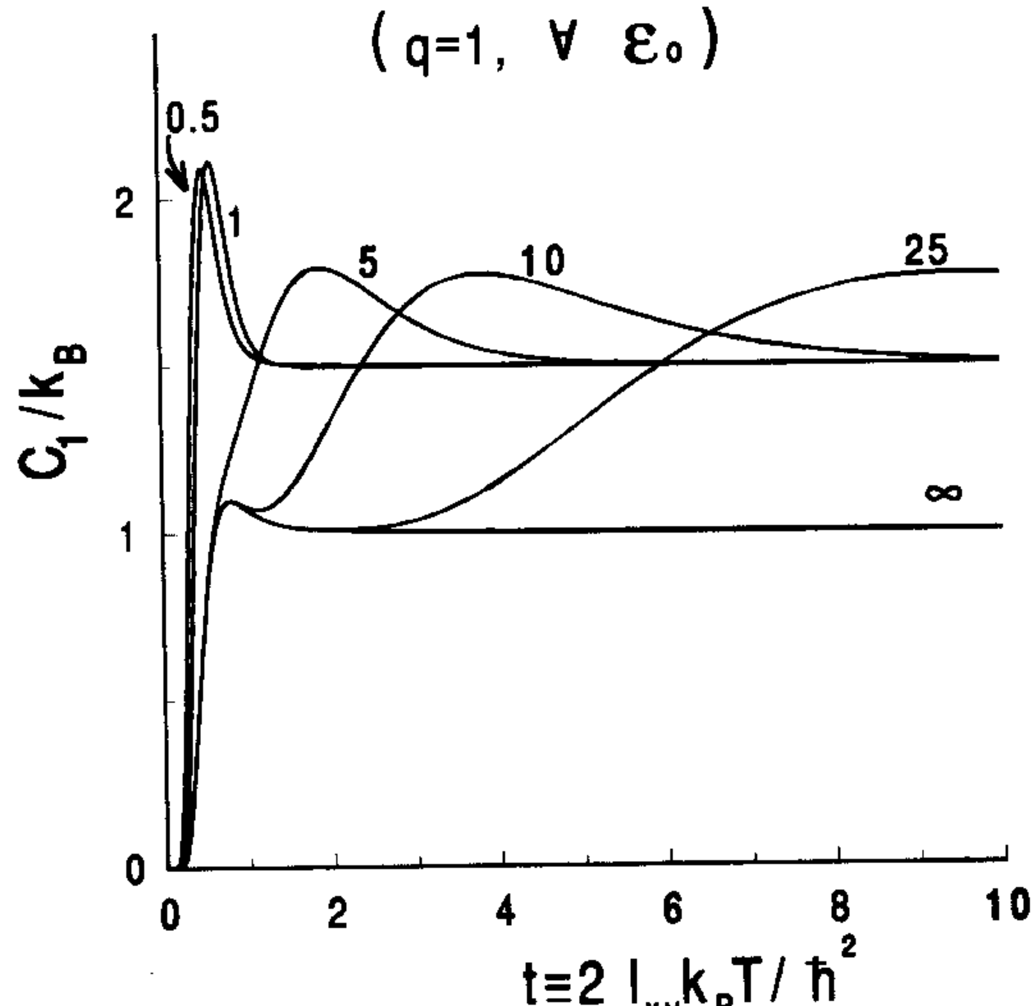


Fig.2a

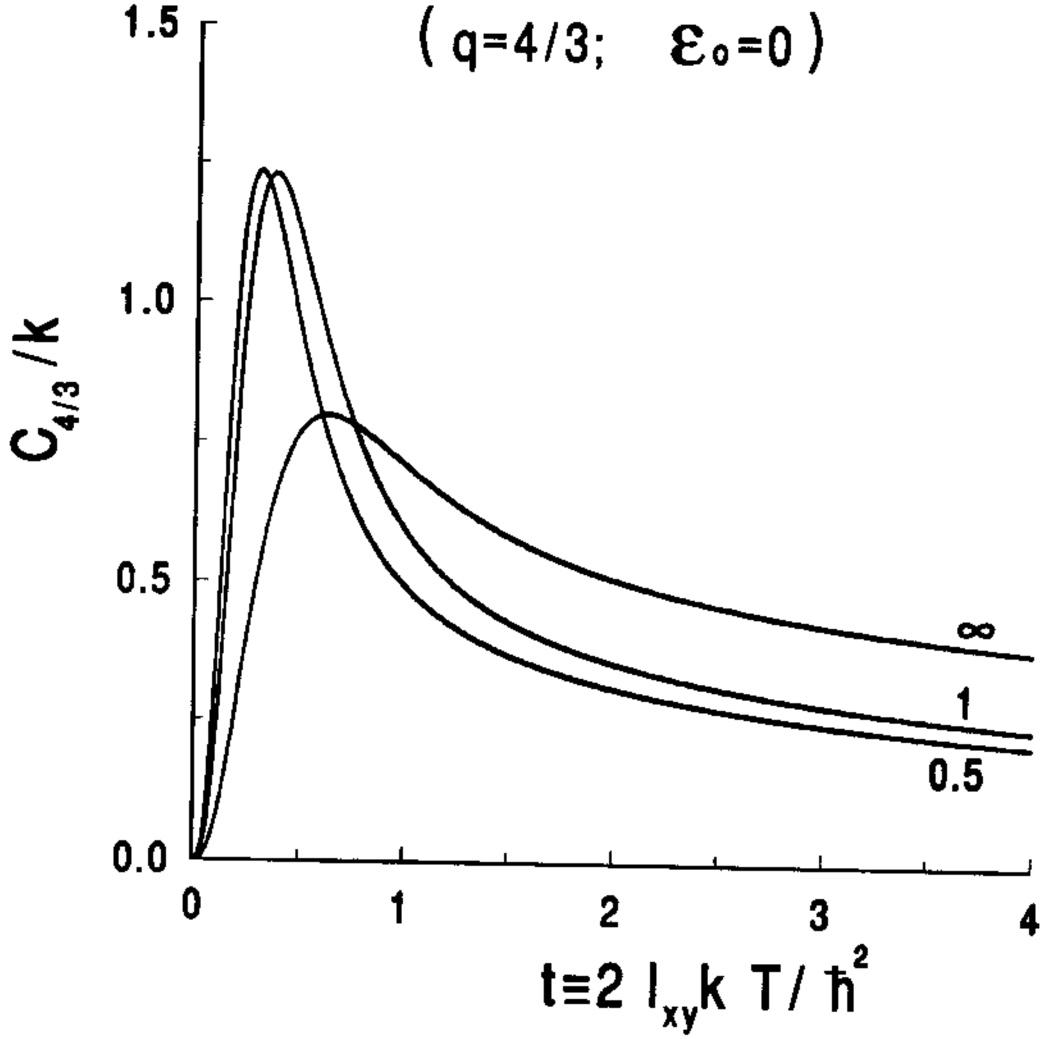


Fig.2b

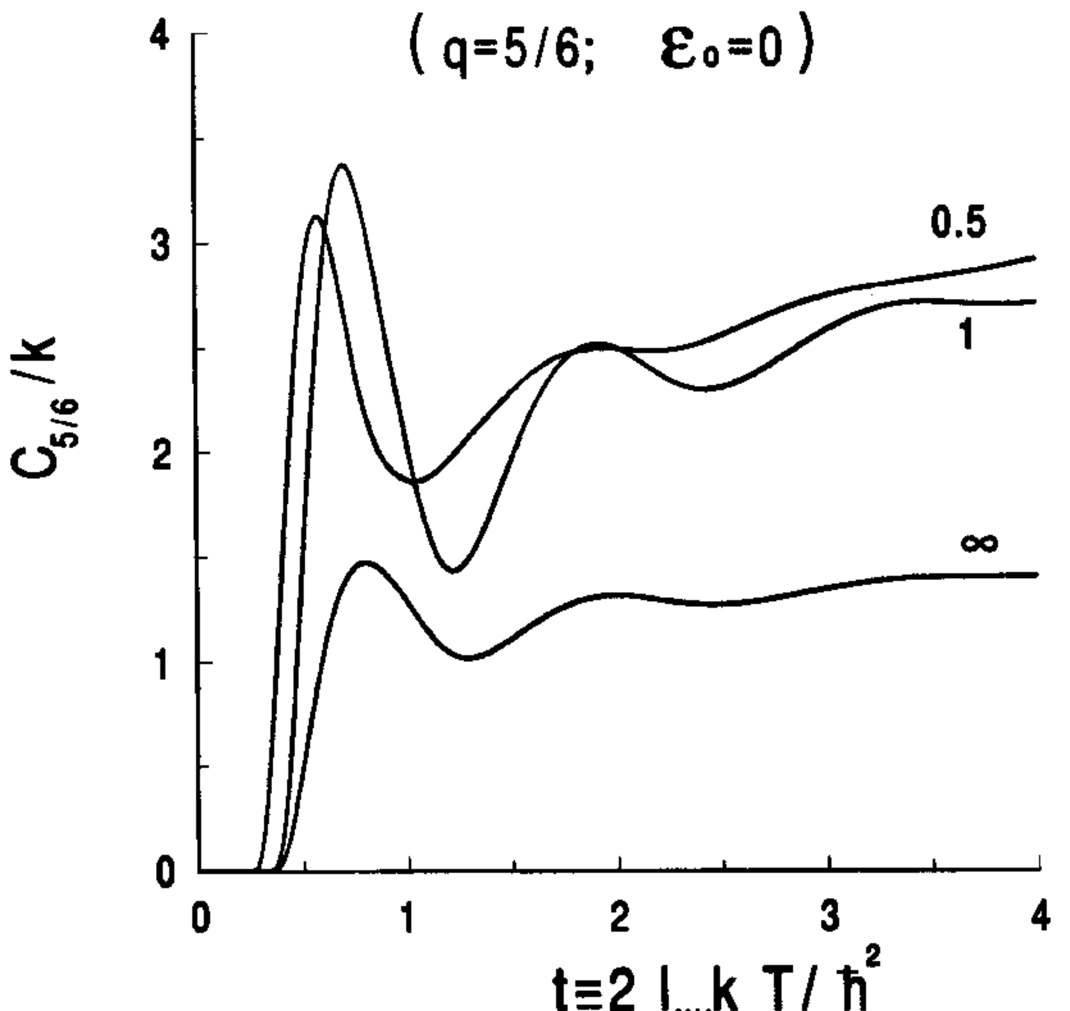


Fig.2c

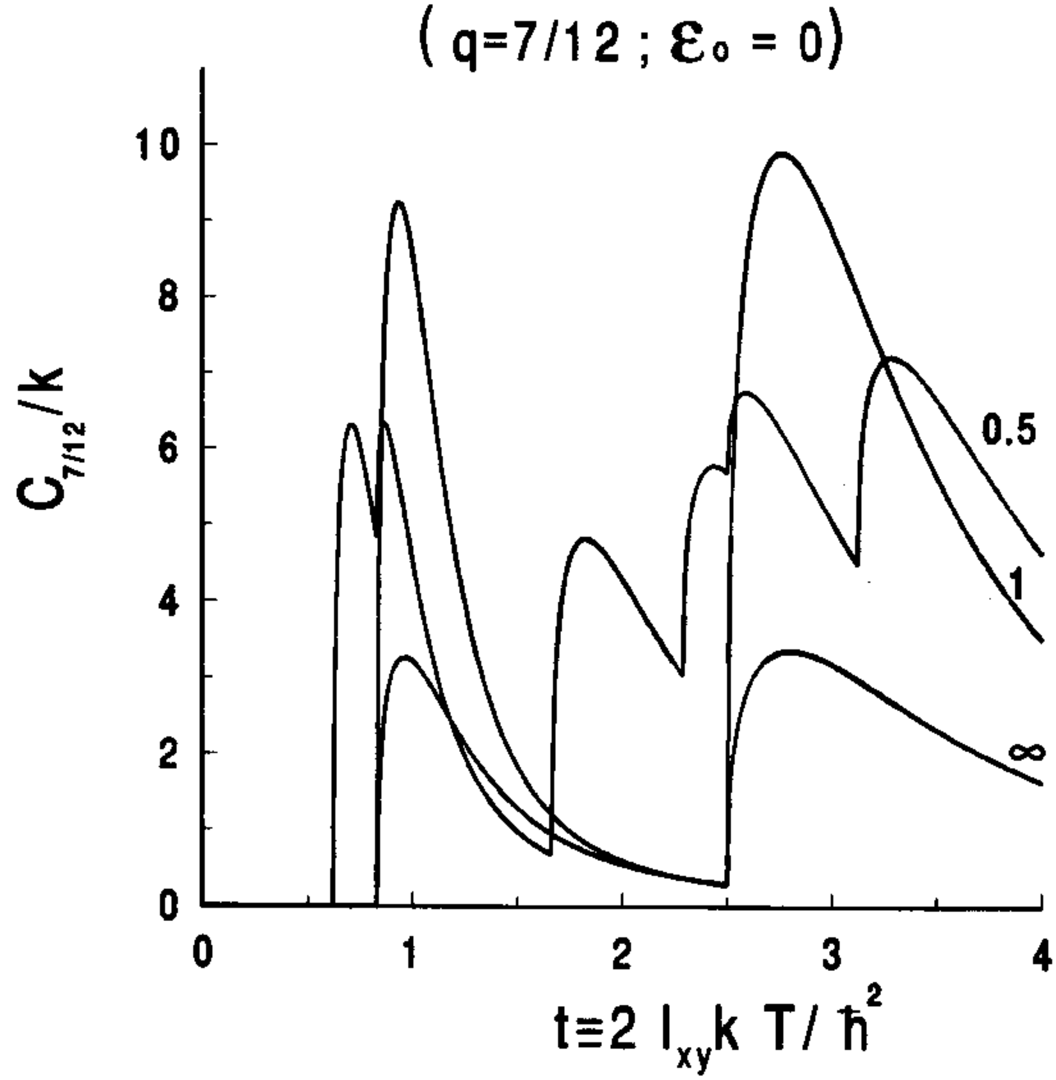


Fig.2d

(q=1/3 ; ε_0= 0)

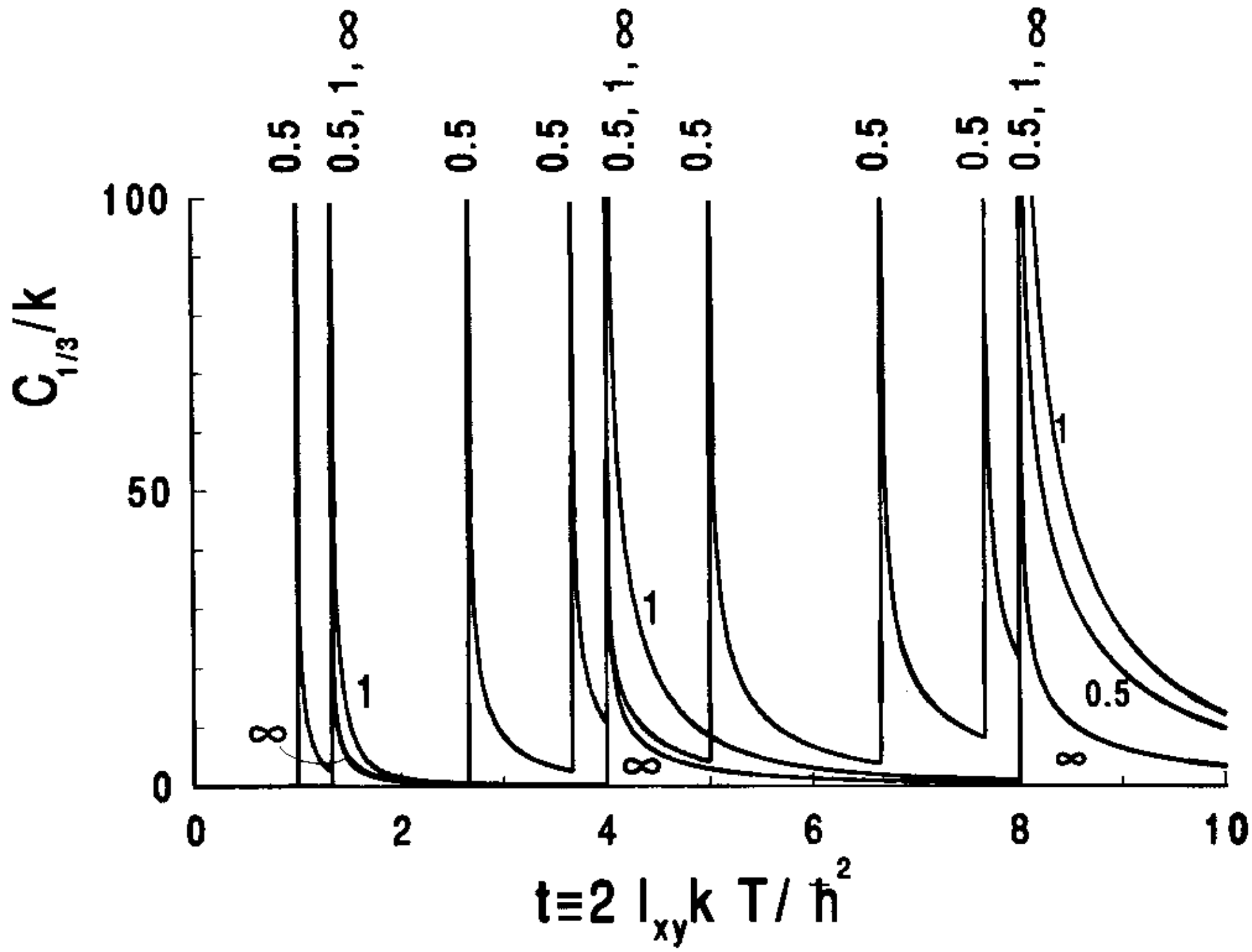


Fig.3a

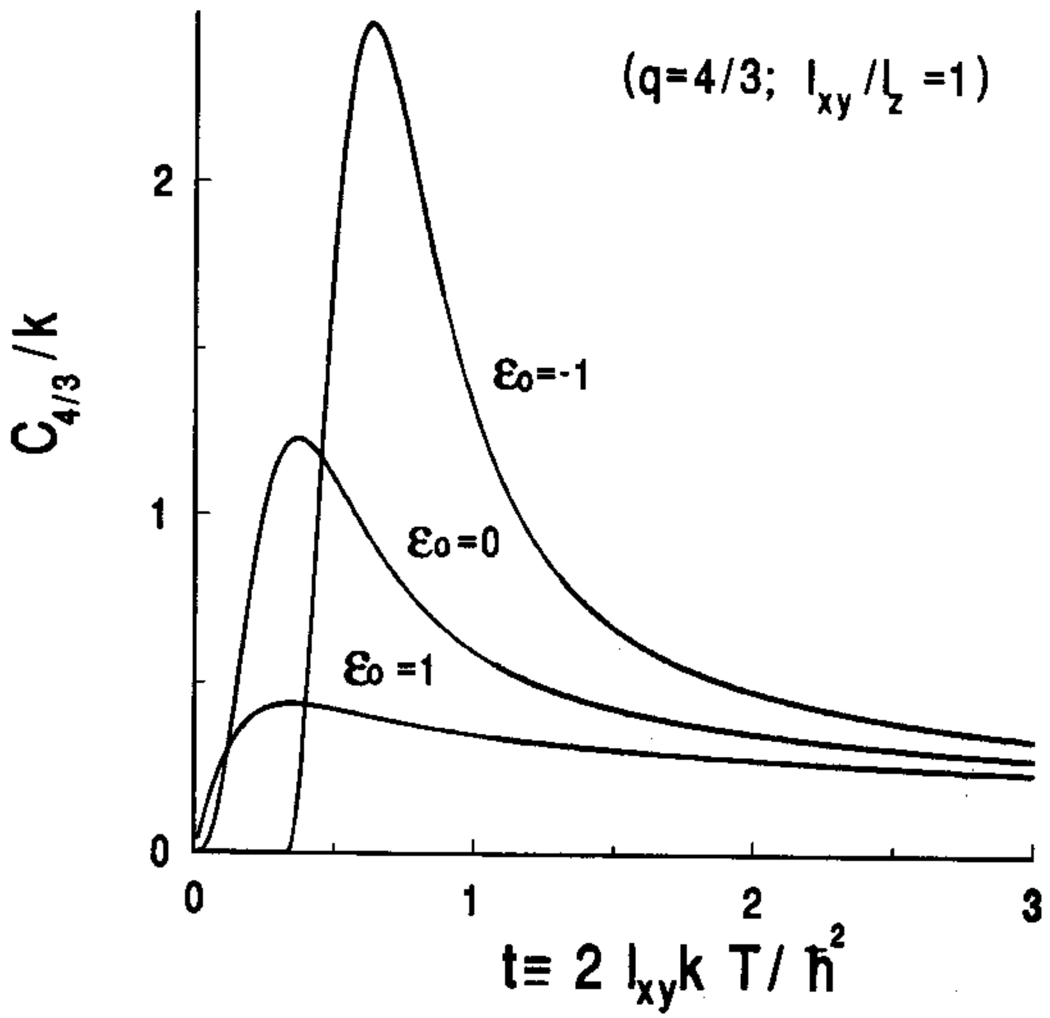
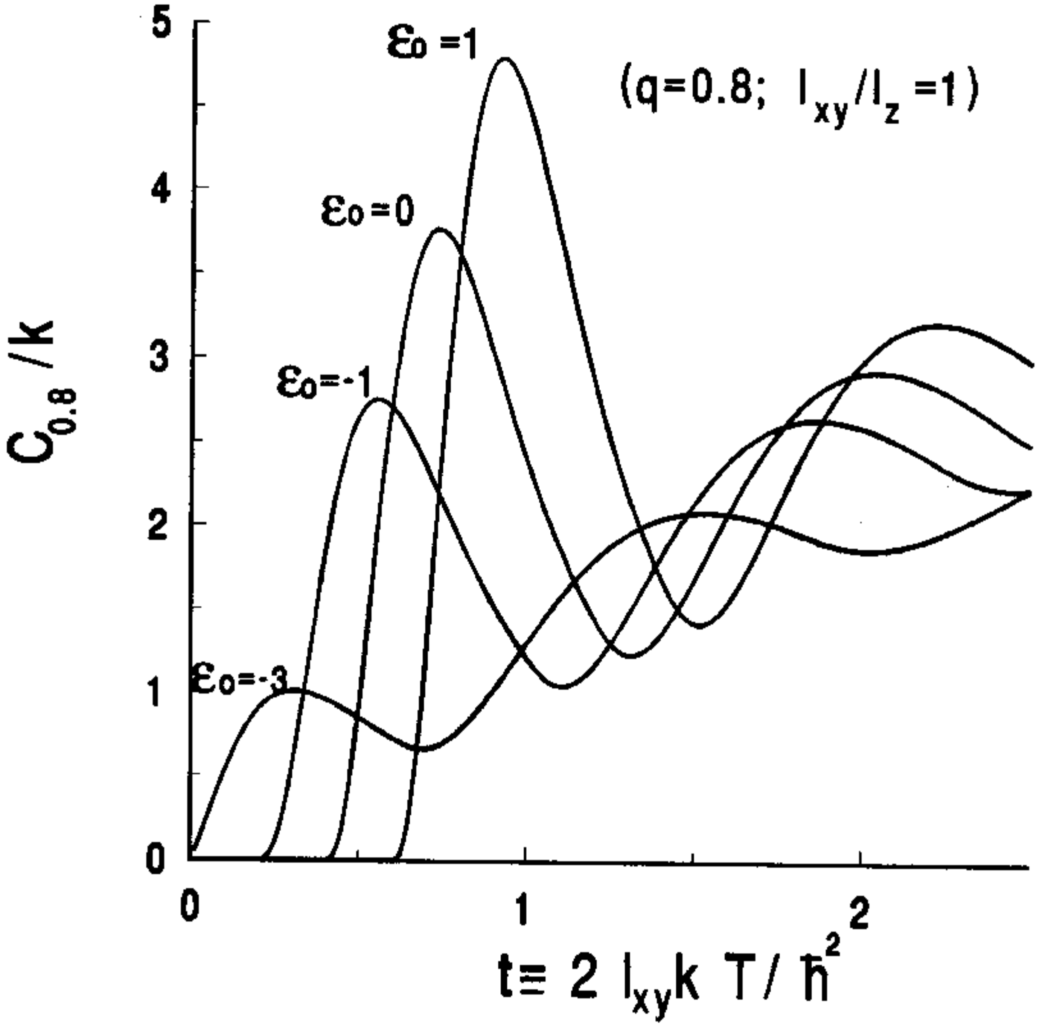


Fig.3b



5
4
3
2
1
0
0
1
2
$C_{0.8}$ /k
t≡ 2 I_{xy}k T/ $\hbar^2$
(q=0.8; I_{xy}/I_z =1)
ε_0 =1
ε_0=0
ε_0=-1
ε_0=-3

Fig.4

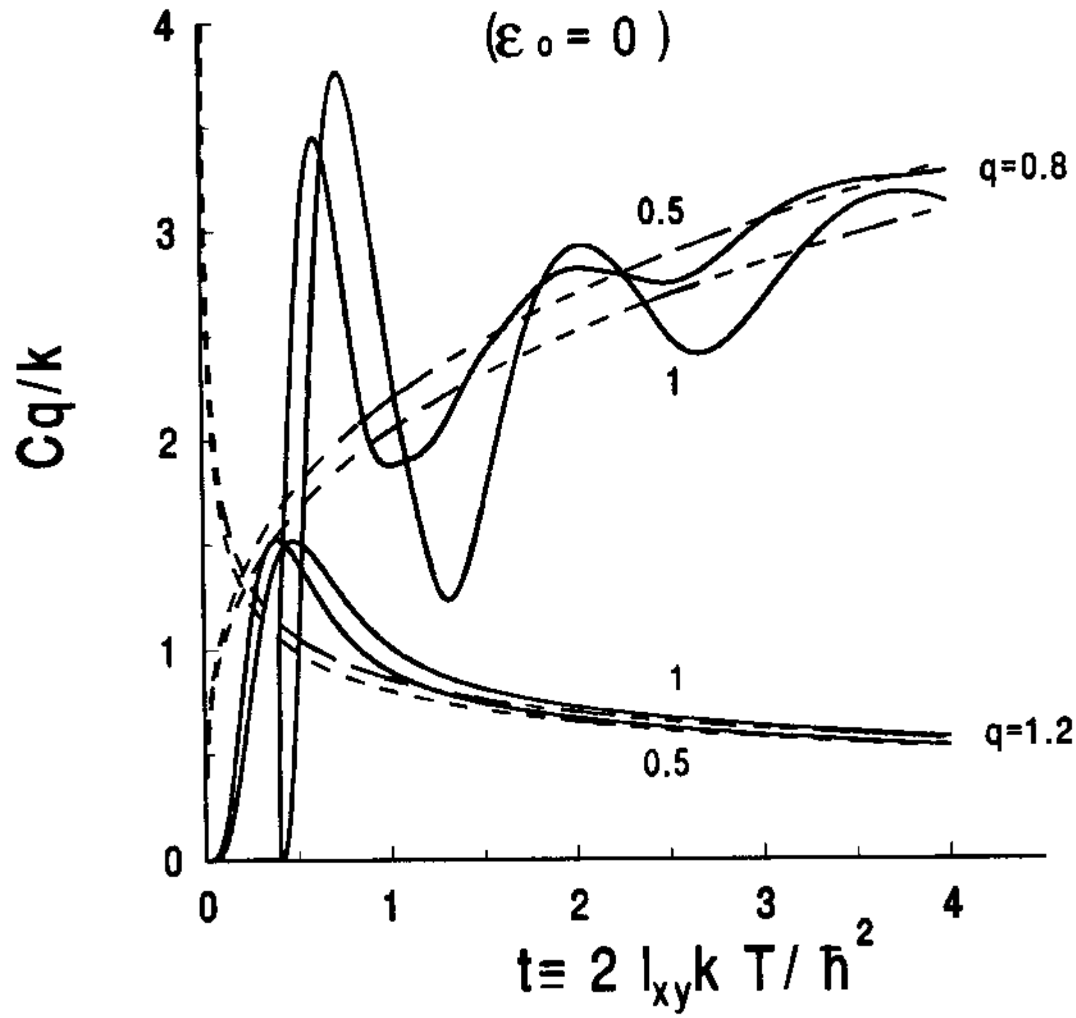


Fig.5a

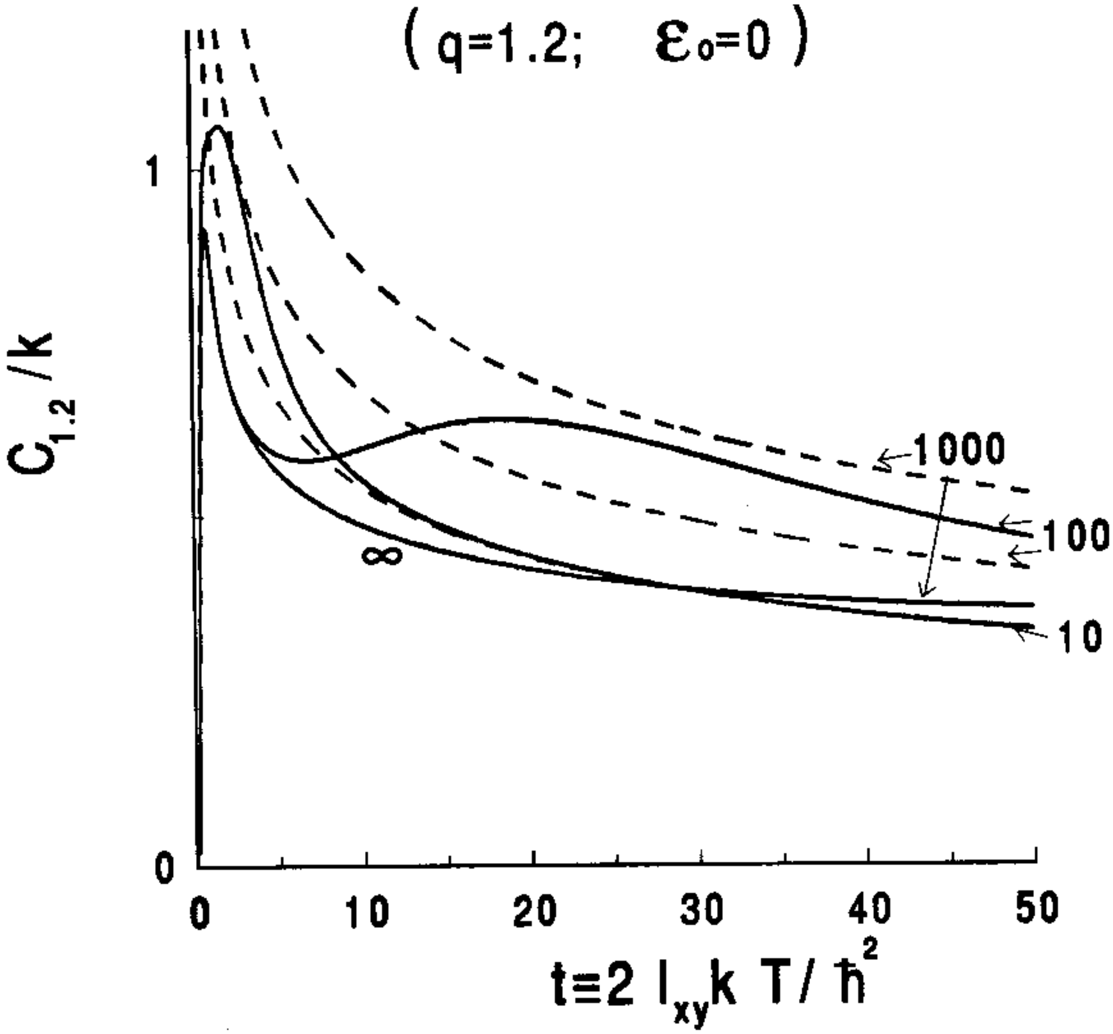
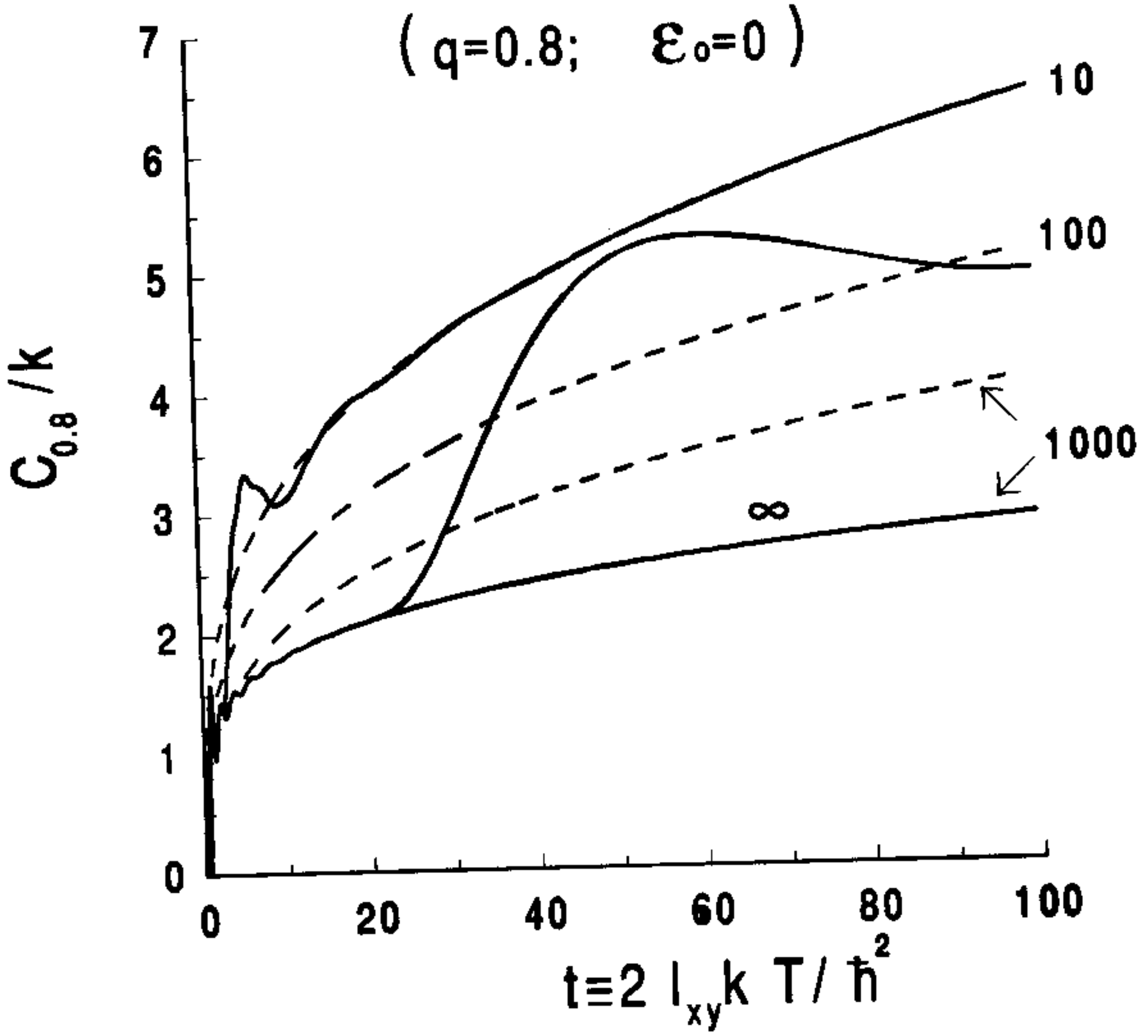


Fig.5b



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