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Low-frequency expansion and specific heat for harmonic chains with random masses

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Abstract. In the problem of harmonic chains with random masses the characteristic function is the analytic continuation into the complex frequency plane of the accumulated density of states and the exponential growth rate. A scheme is developed for the calculation of its asymptotic expansion in powers of the frequency. It is found that it changes sign under the unusual transformation $\omega \to -\omega, \langle\!\langle m^k \rangle\!\rangle \to (-1)^{k-1} \langle\!\langle m^k \rangle\!\rangle$. Its first nine Taylor coefficients are presented in a table. With the first twelve of these coefficients, a two-point Padé approximant for a related function is used for the calculation of the derivative of the specific heat, without making use of the spectral density. These calculations are carried out for several families of mass distributions.

1. Introduction

The chain of harmonic oscillators with random masses has been studied for a long time. Of special importance is the work of Dean (1960, 1961) on the calculation of the spectral density for binary mass distributions. He found very irregular behaviour of this function as soon as the ratio of the heavy and the light mass exceeds the critical value two. Existence of so-called special frequencies, where the spectral density vanishes, has been proven by Hori (1968) and others. In the regions between the special frequencies no regular behaviour of the spectral density is seen; Gubernatis and Taylor (1971) found numerically (for a related model) a detailed behaviour of the density of states for several scales of the coarse graining.

Thermodynamic quantities, like the specific heat, however, have not been calculated, as far as we know. These are smooth functions of the temperature, given by integrals involving the spectral density. Irregular behaviour of this function will not have much influence on them. Calculations of the zero point energy have been carried out by Domb *et al* (1959). In this paper we will calculate the derivative of the specific heat with respect to the temperature. We have chosen this function because it will turn out to be sensitive for the choice of the mass distribution. The method we use is not exact but can be used without much effort for any mass distribution. Its main advantage is the fact that it does not need knowledge of the spectral density. This would be cumbersome, since the integral of this function must be calculated from Schmidt's functional equation (Schmidt 1957), for a given mass distribution and a given value of the frequency. Instead we express the free energy as a sum involving the characteristic function—which is the analytic continuation of the accumulated spectral density into the complex frequency plane—in special points. These happen to lie in a part of the complex frequency plane where this function can be approximated very well by Padé approximants.

In § 2 we introduce a simple scheme for obtaining the expansion of the characteristic function in powers of the (complex) frequency. The coefficients of this expansion are given in terms of cumulants of the mass distribution. The starting point is an equation for a certain analytic function $D(u)$, previously derived (Nieuwenhuizen 1982). From the solution of this equation, the characteristic function follows immediately for (complex) frequency. In § 3 we use these results and the method mentioned above for a numerical calculation of the derivative of the heat capacity with respect to temperature for several families of mass distributions: binary, rectangular, exponential and gamma distributions. Differences between the various cases and the accuracy of the method are discussed.

2. Low frequency expansion of the characteristic function

In this section we introduce a simple scheme for the calculation of the coefficients of the asymptotic expansion of the characteristic function $\Omega(\xi)$ into powers of $\sqrt{\xi}$. For this purpose we assume existence of all the moments of the mass distribution. The characteristic function extends the integrated spectral density $H(\omega^2)$ into the complex $\xi=-\omega^2$ plane. It is defined by (Nieuwenhuizen 1982)

$$\Omega(\xi)=\langle\log m\rangle+\int \log(\xi+\omega^2)\,\mathrm{d}H(\omega^2) \tag{2.1}$$

and has the property

$$\Omega(-\omega^2\pm \mathrm{i}0)=\gamma(\omega^2)\pm \mathrm{i}\pi H(\omega^2). \tag{2.2}$$

The quantity $\gamma(\omega^2)$, defined by the real part of (2.1)–(2.2), was introduced originally by Matsuda and Ishii (1970). It is positive for disordered one-dimensional systems and behaves for small ω^2 as

$$\gamma(\omega^2)=\tfrac{1}{8}(\langle\langle m^2\rangle\rangle/\langle m\rangle)\omega^2 \qquad (\omega^2\downarrow 0), \tag{2.3}$$

where $\langle\langle m^2\rangle\rangle$ is the second cumulant of the mass distribution. Its positivity is connected to the exponential localisation of all eigenfunctions (Matsuda and Ishii 1970, Thouless 1972). Further it is known that as $\omega\downarrow 0$ the integrated spectral density takes the same value as for the chain where all masses have been replaced by their average values, i.e. $H(\omega^2)\to \pi^{-1}(\langle m\rangle)^{1/2}\omega$. Inserting this and (2.3) into (2.2) we obtain

$$\Omega(\xi)=(\langle m\rangle\xi)^{1/2}-\tfrac{1}{8}(\langle\langle m^2\rangle\rangle/\langle m\rangle)\xi \qquad \xi\to 0. \tag{2.4}$$

Now we proceed to the evaluation of the higher-order terms of this expansion. As proven in Nieuwenhuizen (1982), the characteristic function can be obtained for given (complex) value of ξ from a certain function $D(u)$, analytic in u and its implicit variable ξ. This function satisfies the equation

$$D(u)=\int \mathrm{d}R(m)[D(2+m\xi-u^{-1})+\log(2+m\xi-u^{-1})]-D(\infty), \tag{2.5}$$

where $R(m)$ is the common distribution function of the independently distributed masses m_1, m_2, ... The characteristic function follows from the simple identity

(Nieuwenhuizen 1982)

$$\Omega(\xi) = D(\infty). \tag{2.6}$$

For small ξ the behaviour of D is governed by the average value of m. We therefore put

$$m = \langle m\rangle(1+\delta m). \tag{2.7}$$

If we neglect the fluctuations δm, the solution (2.5) is given by (Nieuwenhuizen 1982)

$$D_0(u) = \log(\mathrm{e}^{\mu} - u^{-1}) \tag{2.8}$$

where μ is defined by

$$\cosh\mu = 1 + \tfrac{1}{2}\langle m\rangle\xi, \qquad \sinh\mu = (\langle m\rangle\xi + \tfrac{1}{4}\langle m\rangle^2\xi^2)^{1/2}. \tag{2.9}$$

We introduce a new variable z, such that the singularity of D_0 at $u = \mathrm{e}^{-\mu}$ is mapped onto the origin

$$z = (u\mathrm{e}^{\mu} - 1)/(u\mathrm{e}^{-\mu} - 1). \tag{2.10}$$

Then (2.8) takes the form

$$D_0(u(z)) = \log(2z\sinh(\mu)/(z-1)). \tag{2.11}$$

Returning to the general case, we define a new function E by

$$D(u(z)) = D_0(u(z)) + E(z\,\mathrm{e}^{-2\mu}). \tag{2.12}$$

The characteristic function is given by

$$\Omega = \mu + E(1). \tag{2.13}$$

From (2.5) follows for $E(z)$ the equation

$$E\left(z - \frac{2\eta z}{(1+\frac{1}{2}\eta)^2}\right) = \left\langle E\left(z - \frac{\frac{1}{2}\eta\delta m(z-1)^2}{1+\frac{1}{2}\eta\delta m(z-1)}\right) + \log\left(1 + \tfrac{1}{2}\eta\delta m\left(1 - \frac{1}{z}\right)\right)\right\rangle - E(1), \tag{2.4}$$

where the angular brackets indicate averaging with respect to m; η is defined by

$$\eta = \frac{\langle m\rangle\xi}{\sinh\mu} = [\langle m\rangle\xi/(1+\langle m\rangle\tfrac{1}{4}\xi)]^{1/2}. \tag{2.15}$$

Further we used $\mathrm{e}^{-\mu} = (1-\frac{1}{2}\eta)/(1+\frac{1}{2}\eta)$.

In the following we will need the 'boundary condition' $|E(\infty)| < \infty$, or, equivalently

$$\lim_{z\to\infty} zE'(z) = 0. \tag{2.16}$$

The form of (2.14) is appropriate for expansion in powers of η. In order to demonstrate the method we now calculate Ω up to order η^5. For given integer $N \geq 1$ we expand E as

$$E(z) = \eta E_1(z) + \ldots + \eta^N E_N(z) + R_N(z;\eta) \tag{2.17a}$$

and define

$$E(1) = \eta Z_1 + \ldots + \eta^N Z_N + R_N(1;\eta) \tag{2.17b}$$

Upon substitution into equation (2.14) this yields the equations

$$0=-Z_1 \tag{2.18a}$$

$$-2zE_1' = -\tfrac{1}{2}\delta_2(1-1/z)^2 - Z_2 \tag{2.18b}$$

$$-2zE_2' + 2zE_1' + 2z^2E_1'' = \delta_2(z-1)^3E_1' + \tfrac{1}{2}\delta_2(z-1)^4E_1'' + \tfrac{1}{3}\delta_3(1-1/z)^3 - Z_3 \tag{2.18c}$$

$$\begin{aligned}-2zE_3' + 2zE_2' - \tfrac{3}{2}zE_1' + 2z^2E_2'' - 4z^2E_1'' - \tfrac{4}{3}z^3E_1''' &= \delta_2(z-1)^3E_2' - \delta_3(z-1)^4E_1' \\ &\quad + \tfrac{1}{2}\delta_2(z-1)^4E_2'' - \delta_3(z-1)^5E_1'' - \tfrac{1}{6}\delta_3(z-1)^6E_1''' - \tfrac{1}{4}\delta_4(1-1/z)^4 - Z_4.\end{aligned} \tag{2.18d}$$

Here the δ_k are proportional to the central moments:

$$\delta_k = (2\langle m\rangle)^{-k}\langle(m-\langle m\rangle)^k\rangle \tag{2.19}$$

and $\delta_1=0$. Using (2.16) we can solve the $E_i'(z)$ and Z_i; from (2.18*b*), for instance, it follows immediately that $Z_2=-\tfrac{1}{2}\delta_2$. For the calculation of Z_k ($k\geq 3$), only $E'(z),\ldots,E_{k-2}'(z)$ is needed. We obtain

$$\begin{aligned}E_1'(z) &= \tfrac{1}{4}\delta_2(-2/z^2+1/z^3)\\ E_2'(z) &= \tfrac{1}{2}\delta_2(1/z^2-1/z^3)+\tfrac{1}{8}\delta_2^2(-9/z^2+12/z^3-7/z^4+3/2z^5)\\ &\quad +\tfrac{1}{6}\delta_3(3/z^2-3/z^3+1/z^4)\end{aligned} \tag{2.20}$$

and

$$Z_1=0 \qquad Z_2=-A_1 \qquad Z_3=2A_2-\tfrac{5}{2}A_1^2 \qquad Z_4=-6A_3+18A_2A_1-15A_1^3 \tag{2.21}$$

where A_k is proportional to the $(k+1)$th cumulant of the mass distribution

$$A_k = [1/(k+1)!\,2^{k+1}]\langle\langle m^{k+1}\rangle\rangle/\langle m\rangle^{k+1}. \tag{2.22}$$

The equation for $R_N(z;\eta)$ has the form (2.14) but the inhomogeneous term is different and for fixed value of z proportional to η^{N+1} for small η. Since the solution of equation (2.5) for $D(u,\xi)$ is unique (Nieuwenhuizen 1982) the solution of the homogeneous part of (2.14) vanishes for all z. Thus for small η $R_N(z;\eta)$ must be proportional to η^{N+1} too, showing that the expansions (2.17*a*)–(2.17*b*) are asymptotic in η for fixed value of z. From (2.9), (2.13), (2.15), and (2.17*b*) we have

$$\Omega(\xi) = \log[1+\tfrac{1}{2}\langle m\rangle\xi + (\langle m\rangle\xi+\tfrac{1}{4}\langle m\rangle^2\xi^2)^{1/2}] + \sum_{k=1}^{\infty} Z_k\left(\frac{\langle m\rangle\xi}{1+\langle m\rangle\frac{1}{4}\xi}\right)^{k/2} \tag{2.23}$$

This expansion is equivalent to an asymptotic expansion in the variable $\sqrt{\xi}$, (see equation (3.3)). Inserting (2.21) we cover equation (2.4).

The importance of the present method lies in the fact that it only requires algebraic manipulations, but no integrals appear. In the original derivation of equation (2.3), however, Matsuda and Ishii (1970) had to perform a non-trivial integral†; in another approach, starting from the Green function, Denteneer and Ernst (1983, 1984) use an expansion in powers on the fluctuation δm, given by (2.7), and have to perform multiple integrals. Their result for the first four terms of the expansion of Ω in powers

† From the theory developed in Nieuwenhuizen (1982) this can be understood as follows: these authors solved the analogue of the function $W(u,\omega^2)$ for small ω^2 and used for γ the equation $\gamma(\omega^2)=\int\log|1/u|\mathrm{d}W(u,\omega^2)$, while we solve the function $D(u,\xi)$ and use the simpler identity $\gamma(\omega^2)=\mathrm{Re}\,D(\infty,-\omega^2+\mathrm{i}0)$.

of $\sqrt{\xi}$ agrees with the expression that follows from (2.23):

$$\Omega(\xi) = (\langle m\rangle\xi)^{1/2} - \tfrac{1}{8}\kappa_2\langle m\rangle\xi + (\tfrac{1}{24}\kappa_3 - \tfrac{5}{128}\kappa_2^2 - \tfrac{1}{24})(\langle m\rangle\xi)^{3/2}$$
$$+ (\tfrac{1}{32}\kappa_2 - \tfrac{15}{512}\kappa_2^3 + \tfrac{3}{64}\kappa_2\kappa_3 - \tfrac{1}{64}\kappa_4)(\langle m\rangle\xi)^2 \tag{2.24}$$

where

$$\kappa_j = \langle\langle m^j\rangle\rangle / \langle m\rangle^j.$$

Via (2.2) this equation gives the first corrections to the leading behaviour of $\gamma(\omega^2)$ and $H(\omega^2)$ as $\omega^2 \downarrow 0$. We note that already the term of order $\xi^{3/2}$ in (2.24) is not given correctly by effective medium approaches (Denteneer and Ernst 1983, 1984). In the same way the coefficients $Z_5, \ldots, Z_{12}$ have been calculated, using the computer program 'Schoonschip' for performing the algebraic manipulations. The results for $Z_1, \ldots, Z_9$ are presented in table 1. The results for the gamma distributions (3.15) with $m_0 = 0$ are given in table 2; they were used as a check on the data of table 1. From these tables and equation (2.23) we notice two important features.

(i) Ω is antisymmetrc under the 'parity' transformation $\eta \to -\eta$ (or $\sqrt{\xi} \to -\sqrt{\xi}$, or $\omega \to -\omega$ for complex ω) and $A_k \to (-1)^k A_k$. There does not seem to be a physical interpretation for this transformation, but it can be used as a check on the calculations. Further it is obvious that, because of this symmetry, the expressions take relatively simple forms in terms of the A_k.

(ii) Z_k only contains terms of the form contant $\times A_{n_1} A_{n_2} \ldots A_{nj}$ for which $n_1 + \ldots + n_j = k-1, k-3, \ldots$, but $n_1 + \ldots + n_j \geq 2$ if $k \geq 3$. These two properties can be proven for a particular family of mass distributions. The total number of terms in Z_k, n_k

Table 1. The Taylor coefficients Z_k for $k = 1, \ldots, 9$, expressed in terms of the quantities A_k, defined by (2.22).

$$Z_1 = 0$$
$$Z_2 = -A_1$$
$$Z_3 = 2A_2 - \tfrac{5}{2}A_1^2$$
$$Z_4 = -6A_3 + 18A_2A_1 - 15A_1^3$$
$$Z_5 = -\tfrac{9}{8}A_1^2 + 24A_4 - 84A_3A_1 - 38A_2^2 + 221A_2A_1^2 - \tfrac{1105}{8}A_1^4$$
$$Z_6 = \tfrac{21}{2}A_2A_1 - \tfrac{19}{2}A_1^3 - 120A_5 + 480A_4A_1 + 408A_3A_2 - 1350A_3A_1^2 - 1224A_2^2A_1 + 3390A_2A_1^3 - 1695A_1^5$$
$$\begin{aligned} Z_7 = {} & \tfrac{1}{8}A_1^2 - 57A_3A_1 - \tfrac{197}{6}A_2^2 + \tfrac{1091}{6}A_2A_1^2 - \tfrac{10829}{96}A_1^4 + 760A_6 - 3240A_5A_1 - 2640A_4A_2 + 9780A_4A_1^2 \\ & -1242A_3^2 + 16\,692A_3A_2A_1 - 25\,320A_3A_1^3 + 2524A_2^3 - 34\,503A_2^2A_1^2 \\ & + \tfrac{248\,475}{4}A_2A_1^4 - \tfrac{414\,125}{16}A_1^6 \end{aligned}$$
$$\begin{aligned} Z_8 = {} & -\tfrac{3}{2}A_2A_1 - \tfrac{63}{16}A_1^3 + 360A_4A_1 + 446A_3A_2 - 1327A_3A_1^2 - 1332A_2^2A_1 + \tfrac{6969}{2}A_2A_1^3 - 1695A_1^5 - 5040A_7 \\ & + 25\,200A_6A_1 + 19\,920A_5A_2 - 81\,600A_5A_1^2 + 18\,000A_4A_3 - 133\,680A_4A_2A_1 \\ & + 220\,200A_4A_1^3 - 63\,000A_3^2A_1 - 57\,144A_3A_2^2 + 565\,800A_3A_2A_1^2 - 546\,300A_3A_1^4 \\ & + 171\,432A_2^3A_1 - 994\,380A_2^2A_1^3 + 1322\,160A_2A_1^5 - 472\,200A_1^7 \end{aligned}$$
$$\begin{aligned} Z_9 = {} & -\tfrac{1}{32}A_1^2 + 9A_3A_1 + \tfrac{137}{18}A_2^2 + \tfrac{12\,245}{144}A_2A_1^2 - \tfrac{74\,455}{1152}A_1^4 - 2610A_5A_1 - 3380A_4A_2 + 10\,930A_4A_1^2 \\ & - \tfrac{3633}{2}A_3^2 + 22\,186A_3A_2A_1 - 30\,878A_3A_1^3 + \tfrac{10\,618}{3}A_2^3 - \tfrac{177\,905}{4}A_2^2A_1^2 + \tfrac{303\,751}{4}A_2A_1^4 \\ & - \tfrac{5880\,575}{192}A_1^6 + 40\,320A_8 - 221\,760A_7A_1 - 171\,360A_6A_2 + 768\,600A_6A_1^2 - 150\,480A_5A_3 \\ & + 1222\,560A_5A_2A_1 - 2171\,700A_5A_1^3 - 72\,288A_4^2 + 1107\,936A_4A_3A_1 + 502\,128A_4A_2^2 \\ & - 5362\,344A_4A_2A_1^2 + 5523\,165A_4A_1^4 + 473\,796A_3^2A_2 - 2531\,133A_3^2A_1^2 \\ & - 4600\,224A_3A_2^2A_1 + 18\,985\,374A_3A_2A_1^3 - \tfrac{26\,717\,805}{2}A_3A_1^5 \\ & - 348\,634A_2^4 + 8643\,506A_2^3A_1^2 - \tfrac{121\,782\,417}{4}A_2^2A_1^4 + \tfrac{256\,406\,305}{8}A_2A_1^6 - \tfrac{1282\,031\,525}{128}A_1^8 \end{aligned}$$

Table 2. The Taylor coefficients Z_k for $k=1,\ldots,9$ for gamma distributions with $m_0=0$ and parameter n, defined by (3.15).

$$Z_1=0$$
$$Z_2=-\tfrac{1}{8}N^{-1}$$
$$Z_3=\tfrac{17}{384}N^{-2}$$
$$Z_4=-\tfrac{15}{512}N^{-3}$$
$$Z_5=\tfrac{44\,419}{1474\,560}N^{-4}-\tfrac{9}{512}N^{-2}$$
$$Z_6=-\tfrac{1407}{32\,768}N^{-5}+\tfrac{37}{1024}N^{-3}$$
$$Z_7=\tfrac{62\,410\,727}{792\,723\,456}N^{-6}-\tfrac{274\,229}{3538\,944}N^{-4}+\tfrac{1}{512}N^{-2}$$
$$Z_8=-\tfrac{46\,301}{262\,144}N^{-7}+\tfrac{18\,719}{98\,304}N^{-5}-\tfrac{127}{8192}N^{-3}$$
$$Z_9=\tfrac{26\,630\,337\,641}{56\,855\,166\,218}N^{-8}-\tfrac{730\,522\,213}{1358\,954\,496}N^{-6}+\tfrac{2988\,593}{42\,467\,328}N^{-4}-\tfrac{1}{2048}N^{-2}$$

satisfies the equation

$$n_k=n_{k-2}+p(k-1)-1 \qquad (k\geqslant 2) \tag{2.25}$$

where $p(k)$ is the number of unrestricted partitions of k (Abramowitz and Stegun 1972) and the term-1 enters the RHS because a term of the form constant $\times A_{k-2}$—which contains a contribution proportional to δ_{k-1}, arising only from the logarithm in (2.14)—does not occur. For large k one finds that the n_k grow exponentially fast (Abramowitz and Stegun 1972)

$$n_k\sim(4\pi\sqrt{2k})^{-1}\exp(\pi\sqrt{2k/3}) \qquad (k\to\infty). \tag{2.26}$$

This shows that the method becomes very laborious for large k; the number of different terms in $E_k(z)$ grows even faster and this will limit the maximal number of Z_k's that can be evaluated with a modest amount of computer time.

Finally we note that there exists a great number of different one-dimensional models, which have a similar equation of motion (Alexander *et al* 1981), of which we mention: random Heisenberg spin models, random relaxation models, random electric networks. The expansion given above can be extended directly to these models.

3. Calculation of the specific heat

3.1. The method

The free energy per particle, f, for a harmonic system is given by

$$\beta f=\int \mathrm{d}H(\omega^2)\log 2\sinh(\tfrac{1}{2}\beta\hbar\omega) \tag{3.1}$$

where $\beta=1/kT$. We use units in which $k=\hbar=1$. We want to have an expression for f for which no knowledge of $H(\omega^2)$ is needed. The reason is that this function—being proportional of the jump to the characteristic function across its cut in the complex frequency plane—cannot be approximated easily, except for small values of ω^2, see § 2. Using the product formula $\sinh x=x\prod_{l=1}^{\infty}(1+x^2/l^2\pi^2)$ we obtain from (3.1)

$$\beta f=\log\beta-\tfrac{1}{2}\langle\log m\rangle+\sum_{l=1}^{\infty}(\Omega(\xi_l)-\log\xi_l-\langle\log m\rangle) \qquad \xi_l=(2\pi lT)^2. \tag{3.2}$$

Here we used definition (2.1) and the fact that $\langle\log\omega^2\rangle=-\langle\log m\rangle$, see equations (3.5) and (3.6). Formula (3.2) has been derived before (Maradudin *et al* 1971), but it was not used for actual calculations. It only requires knowledge of $\Omega(\xi)$ for positive values of ξ, where this function has no singularities. Hence it can be approximated there with Padé techniques. Using the method described in the preceding section we have calculated the first twelve coefficients of the asymptotic expansion of the function in powers of $\sqrt{\xi}$:

$$\Omega(\xi)=\sum_{k=1}^{12} C_k(\sqrt{\xi})^k+\mathrm{O}(\xi^{13/2}) \qquad (\xi\downarrow 0). \tag{3.3}$$

The behaviour of Ω for large ξ can be obtained easily from the equality (Nieuwenhuizen 1982)

$$\Omega(\xi)=\left\langle\log\left(2+m_1\xi-\frac{1}{2+m_2\xi-}\,\frac{1}{2+m_3\xi-}\cdots\right)\right\rangle \tag{3.4}$$

where the masses $m_1, m_2, \ldots$ are independent random variables with the same distribution. For large ξ we obtain

$$\Omega(\xi)=\log\xi+\langle\log m\rangle+\frac{2}{\xi}\left\langle\frac{1}{m}\right\rangle-\frac{1}{\xi^2}\left(2\left\langle\frac{1}{m^2}\right\rangle+\left\langle\frac{1}{m}\right\rangle^2\right)$$
$$+\frac{1}{\xi^3}\left(4\left\langle\frac{1}{m}\right\rangle\left\langle\frac{1}{m^2}\right\rangle+\tfrac{8}{3}\left\langle\frac{1}{m^3}\right\rangle\right)+\mathrm{O}\left(\frac{1}{\xi^4}\right). \tag{3.5}$$

This expansion equal to the expansion into moments of the frequency distribution, cf (2.1)

$$\Omega(\xi)=\log\xi-\langle\log\omega^2\rangle+(1/\xi)\langle\omega^2\rangle-(1/2\xi^2)\langle\omega^4\rangle+(1/3\xi^3)\langle\omega^6\rangle+\ldots. \tag{3.6}$$

This point was previously considered by Domb *et al* (1959) who used combinatorial methods for the construction of the moment generating function and calculated the moments up to $\langle\omega^{20}\rangle$ (whereas (3.4) was deduced from a simple algebraic equality (Bellman 1956)).

The derivative of the specific heat with respect to temperature follows from (3.2) and is given by

$$\frac{\mathrm{d}c_v}{\mathrm{d}T}=-\frac{1}{T}\sum_{l=1}^{\infty} g(2\pi l T) \tag{3.7}$$

where

$$g(x)=12x^2\Omega'(x^2)+28x^4\Omega''(x^2)+8x^6\Omega'''(x^2). \tag{3.8}$$

For the calculation of $\mathrm{d}c_v/\mathrm{d}T$, we approximate $g(x)$ by a two-point Padé approximant of the form

$$g_N(x)=\frac{p_1x+p_2x^2+\ldots+p_{N-1}x^{N-1}}{1+q_1x+\ldots+q_{N+1}x^{N+1}}. \tag{3.9}$$

The $2N$ unknown coefficients p_k, q_k are fixed by the requirements that (i) n Taylor coefficients of $g_N(x)$ around $x=0$ agree with the values prescribed by (3.3) and (3.8); (ii) $2N-n$ coefficients of the expansion of $g_N(x)$ into powers of $1/x$ agree with equations (3.5) and (3.8) (the odd coefficients vanish.) This is a two point Padé approximation; an explicit solution exists in the form of determinants (Baker 1975).

In order to reproduce the correct low-temperature behaviour we take, instead of (3.7)†,

$$\frac{\mathrm{d}c_v}{\mathrm{d}T}=-\frac{1}{T}\sum_{l=1}^{\infty}g_N(2\pi lT)+\frac{1}{2\pi T^2}\int_0^{\infty}g_N(x)\,\mathrm{d}x. \tag{3.10}$$

For finite N the integral will have a small, non-vanishing value. Using the Euler–Maclaurin summation formula (Abramowitz and Stegun 1972), we obtain from this equation the asymptotic expansion in powers of T^2

$$\frac{\mathrm{d}c_v}{\mathrm{d}T}=\sum_{k=0}^{n_1}(-1)^k\frac{1}{\pi}(2k+1)^2(2k+2)!\,\zeta(2k+2)C_{2k+1}T^{2k}+\mathrm{O}(T^{2n_1+2}), \tag{3.11}$$

where $\zeta(2k+2)$ is the Riemann zeta function and n_1 is the largest integer less than or equal to $\frac{1}{2}n$. The same result follows if one determines $H(\omega^2)$ from (3.3), i.e. $H(\omega^2)=\Sigma_{k=0}^{\infty}1/\pi(-1)^kC_{2k+1}\omega^{2k+1}$ and performs the integral in (3.1) term by term. The first terms of (3.11) are given by

$$\mathrm{d}c_v/\mathrm{d}T=\tfrac{1}{3}\pi\sqrt{\langle m\rangle}+\tfrac{12}{5}\pi^3(\tfrac{1}{24}-\tfrac{1}{24}\kappa_3+\tfrac{5}{128}\kappa_2^2)\langle m\rangle^{3/2}T^2. \tag{3.12}$$

This shows that for most distributions—and in particular symmetric ones, where $\kappa_3=0$—$\mathrm{d}c_v/\mathrm{d}T$ will *increase* for small temperatures, but we will also encounter an exceptional case, where it *decreases.* For large T we have

$$\frac{\mathrm{d}c_v}{\mathrm{d}T}=\sum_{l=1}^{\infty}\frac{B_{2l}\langle\omega^{2l}\rangle}{(2l-2)!\,T^{2l+1}}=\frac{1}{3T^3}\left\langle\frac{1}{m}\right\rangle-\frac{1}{30T^5}\left(2\left\langle\frac{1}{m^2}\right\rangle+\left\langle\frac{1}{m}\right\rangle^2\right)+\ldots. \tag{3.13}$$

Here B_l are Bernoulli numbers and we have used (3.5) and (3.6).

3.2. *Calculation of the derivative of the specific heat*

We have used the method, described above, for a numerical calculation of $\mathrm{d}c_v/\mathrm{d}T$. For that purpose we fixed the first twelve ($n=12$) Taylor coefficients of $g_N(x)$ at $x=0$ to the values following from (3.3) and (3.8) and further also twelve coefficients ($N=12$) of its expansion in powers of $1/x$. (Choosing $N=n$ turned out to yield no poles of $g_N(x)$ for positive x in almost all cases.) Thus in total 24 relations containing non-trivial information about $g(x)$ are satisfied. The calculations have been performed for the following families of mass distributions:

(i) Binary distributions, where the masses take the values $m=1$ and $m=M\geqslant 1$ with probabilities $\frac{1}{2}$, (see figure 1(a)); for comparison we have also plotted the $M=\infty$ expression, which follows from the frequency spectrum given in (Domb *et al* 1959)

$$\frac{\mathrm{d}c_v}{\mathrm{d}T}=q\delta(T)+\frac{2q^2}{T}\sum_{k=1}^{\infty}p^k\sum_{l=1}^{k}\frac{x^2}{\sinh^2x}\left(\frac{x}{\tanh x}-1\right), \tag{3.14}$$

where

$$x=T^{-1}\sin[\pi l/2(k+1)].$$

† One can can also make a two point Padé approximant for $\mathrm{d}c_v/\mathrm{d}T$ as a function of the temperature—or rather its square which is an even function. This will be less accurate, however, than the method used above, since only the odd C_k's are needed and thus less information is used.

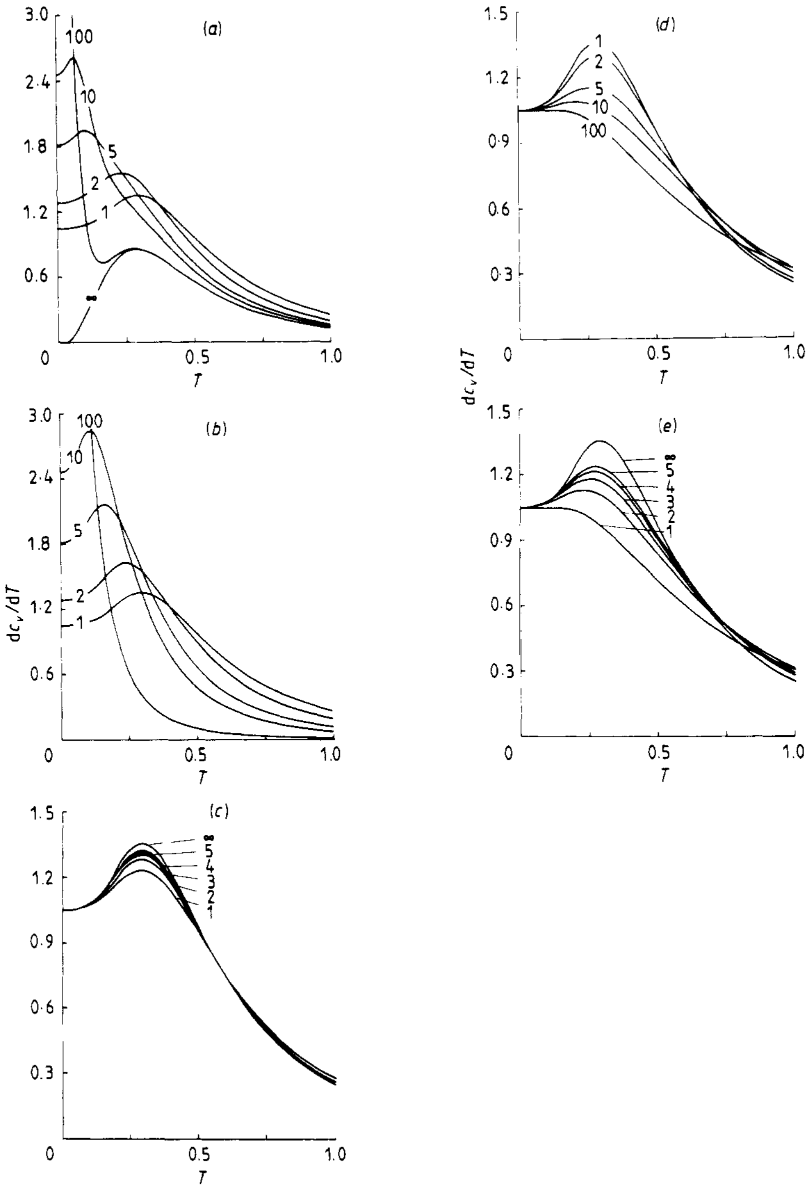

Figure 1. The derivative of the specific heat as a function of temperature for (a) binary distributions ($m = 1$ or $m = M$ with probability $\frac{1}{2}$) for different values of M: (in the case $M = \infty$ there is an additional δ-function at $T = 0$); (b) uniform distributions where $1 \leq m \leq M$ for different values of M; (c) gamma distribution with $m_0 = \frac{1}{2}$ for different values of n, $\langle m \rangle = 1$; (d) exponential distributions for different values of $M = 2/m_0 - 1$, $\langle m \rangle = 1$ and (e) gamma distributions with $m_0 = 0$ for different values of n, $\langle m \rangle = 1$.

Here $p(q)$ is the probability for the occurrence of a light (heavy) particle; we have $p = q = \frac{1}{2}$. Even in the case of mass ratio $M = 100$ the behaviour for low T is quite different from the one predicted by this equation; for high T the agreement is very good. In order to give an idea of the accuracy of our method, we mention that the absolute error is at most equal to 4×10^{-4} if $M=5$, 4×10^{-3} if $M=10$ and 3×10^{-2} in the dip in the case $M=100$. On comparison of the results for different values of $n=N$, the errors seem to decrease exponentially with increasing N. It should be noted that we have calculated the ensemble average of $\mathrm{d}c_v/\mathrm{d}T$. For single, long chains one can also calculate $\mathrm{d}c_v/\mathrm{d}T$. The error due to finite size effects will then be of the order ~ (total number of particles)$^{-1/2}$. Thus for $M=5$ our calculations are as accurate as calculations for a given chain with about $\frac{1}{2}10^7$ particles, which is 20 times larger than the largest chain discussed by Dean (1972).

(ii) Uniform mass distributions where the masses take values between $m=1$ and $m=M\geq1$, (see figure 1(*b*).) As in case (i) $\mathrm{d}c_v/\mathrm{d}T$ increases for low T faster than in the ordered case $M=1$, cf (3.12). If $M\to\infty$ there are essentially no light particles in the system and $\mathrm{d}c_v/\mathrm{d}T$ will approach a δ-function at $T=0$. Also here this approach is slow for low T and fast for large T.

(iii) Distributions where

$$m=m_0+(1-m_0)x \tag{3.15a}$$

with fixed m_0 ($0\leq m_0\leq1$) and the positive random variable x has a gamma distribution with density

$$n\mathrm{e}^{-nx}(nx)^{n-1}/\Gamma(n). \tag{3.15b}$$

In figure 1(*c*) we have taken $m_0=\frac{1}{2}$. The average value of the masses is normalised to unity, so $\mathrm{d}c_v/\mathrm{d}T$ equals $\frac{1}{3}\pi$ at $T=0$, cf (3.12). The second term of this equation is equal to $\frac{12}{5}\pi^3\{\frac{1}{24}+n^{-2}[\frac{5}{128}(1-m_0)^4-\frac{1}{12}(1-m_0)^3]\}T^2$, which is *smaller* than in the ordered case obtained by putting either $m_0=1$ or $n=\infty$ (whereas it is *larger* in cases (i) and (ii)). This indicates that for these distributions the value of $\mathrm{d}c_v/\mathrm{d}T$ will be smaller than in the corresponding ordered model over a large interval, cf figure 1(*c*).

(iv) Exponential distributions where $m_0\leq m<\infty$ ($0\leq m_0\leq1$) with density $(1-m_0)^{-1}\exp[-(m-m_0)/(1-m_0)]$. Here we chose the same ratios for the quantity $M=2\langle m\rangle/m_0-1=2/m_0-1$ (or, equivalently, for the quantity $m_0/\langle m\rangle$) as in the cases (i) and (ii), see figure 1(*d*). For these distributions an exact expression for the characteristic function has been derived (Nieuwenhuizen 1983) and this could be used to test the accuracy of the method. For $m_0\geq0.15$ the absolute error was less than or equal to 1.5×10^{-4}; for the case $m_0=\frac{2}{101}(M=100)$ the exact expression of the accumulated density of states had to be used, because of singularities occurring in $g_N(x)$ for positive x.

(v) For comparison, we have plotted in figure 1(*e*) $\mathrm{d}c_v/\mathrm{d}T$ for gamma mass distributions, with densities as discussed in (iii), with now, however, $m_0=0$. In these cases there is more disorder than in (iii), i.e. the cumulants have larger values. These results have been calculated from values for $H(\omega^2)$ obtained numerically by solving certain differential equations, which follow from (2.5) for these mass distributions (Nieuwenhuizen 1983). The case $n=1$ coincides with the case $m_0=0$ in (iv). Also here in the limit $n=\infty$ all masses have the same value $m=1$, but the approach to this behaviour is much slower than in (iii).

From the $1/n$ expansion, we obtain for the case $m_0=0$ (it also follows from (2.21)–(2.23))

$$\Omega(\xi)=\log(1+\tfrac{1}{2}\xi+\sqrt{\xi+\tfrac{1}{24}\xi^2})-\frac{1}{8n}\frac{\xi}{1+\frac{1}{4}\xi}+\mathrm{O}\left(\frac{1}{n^2}\right). \tag{3.16}$$

This yields a correction to $\mathrm{d}c_v/\mathrm{d}T$ of the form

$$\frac{\mathrm{d}c_v(T;n)}{\mathrm{d}T}=\frac{\mathrm{d}c_v(T;\infty)}{\mathrm{d}T}-\frac{\beta^3}{n\sinh^2\beta}\left\{\left(\frac{\beta}{\tanh\beta}-1\right)^2-\frac{\beta}{2\sinh^2\beta}\left(\tfrac{1}{2}\sinh 2\beta-\beta\right)\right\}+\mathrm{O}\left(\frac{1}{n^2}\right). \tag{3.17}$$

For $T\to\infty$ this coincides with (3.13) in leading order $1/n$. For $T\to 0$ the term proportional to $1/n$ vanishes exponentially fast, which agrees with the fact that there are no contributions proportional to $1/n$ to the odd C_k's, see §§ 2, and 3.1. At $T=0.3$ the correction term is equal to $-0.726/n$, which shows a very slow approach as function of n to the $n=\infty$ value at this temperature.

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