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NUMERICAL COMPUTATION OF THE THERMODYNAMIC PROPERTIES OF THE ORDERED DIATOMIC LINEAR CHAIN

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Synopsis

After a short reminder of the analytical treatment of the main thermodynamic properties of the ordered diatomic linear chain, we give complete numerical results, as well as effective Debye temperature curves, for nine values of the mass-ratio. Comparison with Blackman's specific heat curve and Debye temperature reveals serious deficiencies of the latter.

Résumé

Après un bref rappel du traitement analytique des principales propriétés thermodynamiques de la chaine linéaire diatomique ordonnée, nous donnons les résultats numériques complets, ainsi que les courbes de la température effective de Debye, pour neuf valeurs du rapport de masse. La comparaison avec les courbes de chaleur spécifiqie et de température de Debye obtenues par Blackman révèle de sérieuses erreurs dans le travail de ce dernier.

Introduction

The knowledge of the exact thermodynamic properties of monoatomic and diatomic linear chains is of a great interest in many physical questions. For example, the specific heat of fibrous solids such as Se, Te, HI, etc., was successfully interpreted by Tarasov [1] and de Sorbo [2] by means of a chain-like crystalline model. They, however, considered the chains in the continuum Debye approximation and it seems that an exact atomic treatment

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leads to somewhat different values of the characteristic temperatures of longitudinal vibrations. On an other hand, the exact thermodynamic properties of the ordered diatomic linear chain may serve as a term of comparison in the theory of disordered crystals and may eventually lead to an evaluation of the magnitude of the effect of the isotope mixing by the application of the general theory to this particular case.

To our knowledge, only two works were devoted to the numerical treatment of the thermodynamic properties of unidimensional crystals : Blackman [3] computed the specific heat of monoatomic and diatomic linear chains in order to test the validity of the Debye approximation and more recently J. PIRENNE and P. RENSON [4] gave a full analytical treatment of the main thermodynamic properties of the monoatomic linear chain. This last work reveals the real insufficiency of BLACKMAN's one where the specific heat at low temperature is erroneous by some 17 %.

Presuming that the treatment of the diatomic chain might be affected, in BLACKMAN's work, by the same kind of error, and considering the interest of the question, we undertook a detailed analytical treatment of the thermodynamic potential, energy, entropy and specific heat of the diatomic ordered linear chain following methods similar to that of J. PIRENNE and P. RENSON. In a paper to appear in Physica [5] and hereafter referred to as (B) we gave the detailed analytical developments leading to four series of expansions : a general one, converging at all temperatures and three better expansions adapted to the high, intermediate and low temperature ranges. We also gave typical numerical results and diagrams for a mass ration = 3 showing again serious disagreements with BLACKMAN's numerical integration especially at low temperature.

In the present paper we wish to present our complete numerical results and diagrams for 9 values of the mass ration and for 11 values of the temperature. We evaluated the four main thermodynamic functions by means of a new class of transcendent functions which is a more general case of the transcendent functions met by J. PIRENNE and P. RENSON in their study of the monoatomic chain. We also present numerical tables of a function of the mass ratio and of various integrals of elliptic type met in our precedent paper. All these results will be given after a short reminder of the way leading to the usefull expansions.

The free energy, the energy, the entropy and the specific heat of an ordered diatomic chain are obtained by multiplying the frequency distribution function by the corresponding thermodynamic functions of the harmonic oscillator of frequency ω and by integrating over ω. These quantities may be expressed in terms of the fundamental units $\hbar\omega_m/\pi$ for F and E and the BOLTZMAN constant k for S and C (ω_m is the upper limit of the frequency distribution). If we choose the suitable reduced temperature

$$t = \frac{\pi k \mathrm{T}}{\hbar\omega_m} \tag{1}$$

the reduced quantities $\mathscr{F}$, $\mathscr{E}$, $\mathscr{S}$, $\mathscr{C}$ obey the conventional thermodynamic relations $\mathscr{F} = \mathscr{E} - t\mathscr{S}$, $\mathscr{C} = d\mathscr{E}/dt$, etc. Moreover it is possible to separate the classical limit to which these functions tend at high temperature from the quantum deviations which become important only at low temperature. We have thus

$$\mathrm{F}(\alpha, \mathrm{T}) = \mathrm{N}.\frac{\hbar\omega_m}{\pi}, [\mathscr{F}_c(\alpha, t) + \Delta_q\mathscr{F}(\alpha, t)] \tag{2a}$$

$$\mathrm{E}(\alpha, \mathrm{T}) = \mathrm{N}.\frac{\hbar\omega_m}{\pi}, [\mathscr{E}_c(\alpha, t) + \Delta_q\mathscr{E}(\alpha, t)] \tag{2b}$$

$$\mathrm{S}(\alpha, \mathrm{T}) = \mathrm{N}.k.\,[\mathscr{S}_c(\alpha, t) + \Delta_q\mathscr{S}(\alpha, t)] \tag{2c}$$

$$\mathrm{C}(\alpha, \mathrm{T}) = \mathrm{N}.k.\,[\mathscr{C}_c(\alpha, t) + \Delta_q\mathscr{C}(\alpha, t)] \tag{2d}$$

where α is a dimensionless parameter defined by

$$\alpha = \frac{\mathrm{M} - m}{\mathrm{M} + m} \tag{3}$$

function of the masses of the heavy and light atoms M and m.

As shown in (B), the integrals appearing in the evaluation of the classical limits are all trivial except

$$\varkappa(\alpha) = \int_{\mathscr{D}} lgx.\,\frac{(2x^2 - 1)}{\sqrt{(1 - x^2)\,(2x^2 - 1 - \alpha)\,(2x^2 - 1 + \alpha)}}\,dx \tag{4}$$

with $x = \dfrac{\omega}{\omega_m}$ and $\mathscr{D}$ defined by $0 \leqslant x \leqslant \sqrt{\dfrac{1-\alpha}{2}}$ and $\sqrt{\dfrac{1+\alpha}{2}} \leqslant x \leqslant 1$ the two parts of the interval corresponding to the acoustical and

optical branches of the vibration spectrum of the diatomic chain. We shall expose how we did compute this integral in the second part of this paper.

On the other hand, it is shown in (B) how the quantum deviations can easily be expressed in terms of the transcendant functions.

$$\sigma(\alpha, \tau) = \frac{\tau}{\pi} \int_{\mathscr{D}} lg \frac{Sh\left(\frac{\pi x}{\tau}\right)}{\left(\frac{\pi x}{\tau}\right)} \cdot \frac{(2x^2 - 1)}{\sqrt{(1-x^2)(2x^2-1-\alpha)(2x^2-1+\alpha)}} dx \quad (5a)$$

$$\sigma_{1/2}(\alpha, \tau) = \tau^2 \frac{d}{d\tau}\left[\frac{\sigma(\alpha, \tau)}{\tau}\right] \quad (5b)$$

$$\sigma_{3/2}(\alpha, \tau) = \left[\tau . \frac{d}{d\tau} \cdot - 1\right] \sigma_{1/2}(\alpha, \tau) \quad (5c)$$

where $\tau = 2t$.

The problem of evaluating the thermodynamic functions is thereby reduced to the evaluation of the σ functions. This task may be carried out by different expansions of (5a). Immediately (5b) and (5c) give the expression of $\sigma_{1/2}$ and $\sigma_{3/2}$.

If we first develop $Sh\left(\frac{\pi x}{\tau}\right)$ in series of powers of $\frac{1}{\tau}$ we obtain

$$\sigma(\alpha, \tau) = \tau \sum_{n=1}^{\infty} \frac{1}{2} lg \frac{2n\tau\sqrt{1 + n^2\tau^2} + \sqrt{(1 + 2n^2\tau^2)^2 - \alpha^2}}{4n^2\tau^2} \quad (6)$$

This expansion is convergent for all positive value of τ. The computation of this series would however require a great number of terms especially at low ($\tau \leqslant 0{,}25$) and intermediate ($0{,}25 \leqslant \tau \leqslant 2$) temperature.

But even at high temperature ($\tau \geqslant 2$) we found a series more rapidly convergent than (6) and which correspond to an evaluation by the moments method of THIRRING's formula. We had thus

$$\sigma(\alpha, \tau) = -\frac{\tau}{\pi} \sum_{n=1}^{\infty} (-1)^n \cdot \frac{1}{1 + \alpha} [4(V_{n+1} - \sum_{j=0}^{n+1} (-1)^{j+1} \binom{n+1}{j} V_j)$$

$$- 2(V_n - \sum_{j=0}^{n} (-1)^j \binom{n}{j} V_j)] \frac{1}{2n} \cdot \zeta(2n) \cdot \frac{1}{\tau^{2n}} \quad (7)$$

where the V_j are given by recurrence relations that we shall give in our second §. This expansion is convergent for $\tau > 1$.

In the intermediate temperature range we took the 10 first terms of (6) and we evaluated the rest of the series by a method similar to that by which we established the expansion (7). We obtained

$$\sigma(\alpha, \tau) = \tau \sum_{n=1}^{10} \frac{1}{2} \cdot lg \frac{2n\tau\sqrt{1 + n^2\tau^2} + \sqrt{(1 + 2n^2\tau^2)^2 - \alpha^2}}{4n^2\tau^2}$$

$$- \frac{\tau}{\pi} \sum_{n=1}^{\infty} (-1)^n \frac{1}{1 + \alpha} [4(V_{n+1} - \sum_{j=0}^{n+1} (-1)^{j+1} \binom{n+1}{j} V_j)$$

$$- 2(V_n - \sum_{j=0}^{n} (-1)^j \binom{n}{j} V_j)] \frac{1}{2n} \cdot \zeta_{10}(2n) \cdot \frac{1}{\tau^{2n}} \tag{8}$$

with

$$\zeta_q(2n) = \sum_{m=q+1}^{\infty} \frac{1}{m^{2n}} \tag{9}$$

We shall give further a table of this partial Riemanian function. The expression (8) is convergent for $\tau > 1/(q + 1)$.

For lower temperatures, we established an asymptotic development of the contribution of the acoustical branch of $\mathscr{F}(\alpha, t)$, the optical branch contribution being of the singular exponential type and for this reason bringing no contribution to the low temperature asymptotic expansion. We had thus

$$\mathscr{F}(\alpha, \tau) \approx \frac{\varepsilon_0 . \pi}{\hbar\omega_m} + \left[\sum_{s=n+m+p+2}^{\infty} \sum_{s=n+m+p+1}^{\infty} \right] (-1)^s$$

$$\binom{\frac{1}{2}}{n} \binom{\frac{1}{2}}{m} \binom{\frac{1}{2}}{p} \frac{1}{b^{2m+1} c^{2p+1}} \cdot \frac{B_s}{2s(2s - 1)} \cdot \tau^{2s} \tag{10}$$

where ε_0 is the zero point energy per atom and B_s are the BERNOUILLI's numbers. The other fucntions $\mathscr{E}$, $\mathscr{S}$, $\mathscr{C}$ are obtained by the traditional thermodynamic relations.

The computation of the transcendant functions $\sigma(\alpha, \tau)$, $\sigma_{1/2}(\alpha, \tau)$, $\sigma_{3/2}(\alpha, \tau)$ and of the thermodynamic functions $\mathscr{F}(\alpha, t)$, $\mathscr{E}(\alpha, t)$, $\mathscr{S}(\alpha, t)$ and $\mathscr{C}(\alpha, t)$ was carried out with the aid of the electronic computer Bull Gamma ET of the « Centre de Calcul » of this University to a precision of 10^{-5}. We used the series (7) for the high temperature range ($\tau \geqslant 2$), the series (8) in the intermediate temperature range ($0{,}25 \leqslant \tau \leqslant 2$) and the asymptotic expansion (9) in the low temperature range ($\tau \leqslant 0{,}25$). We established tables of these seven functions for values of the α parameter varying from 0.1 to 0.9 by step of 0.1 and for 11 values of the temperature included in

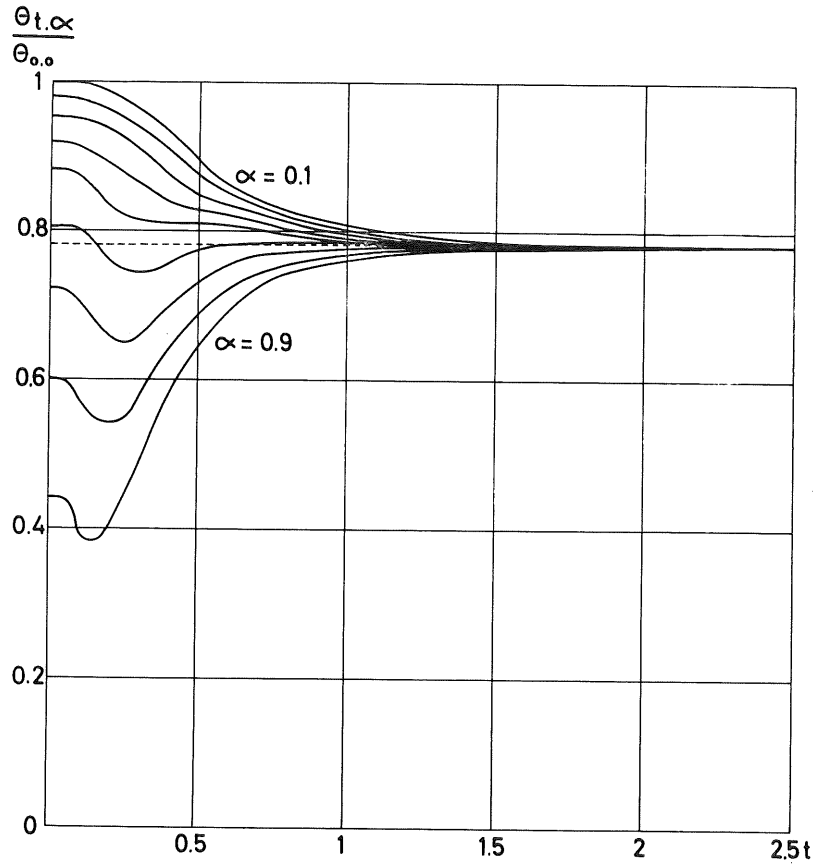

Fig. 4. — Relative effective DEBYE temperature $\Theta_{t.\alpha}/\Theta_{0.0}$ versus t, of the diatomic chain for nine values of the α parameter

$0 \leqslant \tau \leqslant 5$. The diagrams 1, 2, 3 and the tables 1 to 7 give our results. By means of the numerical values of $\mathscr{C}(\alpha, t)$ we established the curves of the Debye characteristic temperature versus t. They are shown in figure 4.

The integral (4) does not seem to be reductible to known transcendant functions and we were lead to evalute it by numerical integration. We used the GAUSS formula

$$\int_{-1}^{+1} f(x) \cdot dx = \sum_{j=1}^{n} \mathrm{H}_j \cdot f(a_j) \tag{11}$$

where the a_j are the roots of the Legendre polynomial of degree n. The H_j are statistical weights affecting the values of the function at the different points of partition of the interval. For a complete discussion of this method see reference [6].

We integrated our function analytically at each limit of both acoustical and optical intervals on a width of 1/1000 of the interval. Owing to the fact that we had only at our disposal the values of the a_j up to $n = 16$ [7] and in order to reach a sufficient precision we were obliged to divide both intervals in two half intervals and taking $n = 16$ in each one we had thus 32 points of division for each branch. The values of this integral are collected in table 8.

The V_j functions apperaring in the high and intermediate temperature expansions are defined by

$$\mathrm{V}_j = \int \frac{du}{(1 + k \cdot sn^2 u)^j} \tag{12}$$

They are given by the recurrence relations

$$\mathrm{V}_0(k) = \mathrm{K}(k)$$

$$\mathrm{V}_1(k) = \frac{1}{4(1+k)} [\pi + 2(1+k)\,\mathrm{V}_0]$$

$$\mathrm{V}_2(k) = \frac{1}{2k(1+k)^2} [k.\mathrm{E}(k) + k(1+k)\,\mathrm{V}_0 + (2k^3+4k^2+2k)\mathrm{V}_1]$$

$$\mathrm{V}_{m+3}(k) = \frac{1}{4(m+1)k(1+k)^2} [(2m-5)k^2\mathrm{V}_m - (2m-4)(k^3+3k^2+k)\mathrm{V}_{m+1} + (2m-3)\,(k^3+2k^2+k)\mathrm{V}_{m+2}] \tag{13}$$

where $K(k)$ and $E(k)$ are the complete elliptic functions of first and second kind. The parameter k, which is known as the « modulus » in the theory of elliptic integrals has of course nothing to do with the BOLTZMAN constant and is defined by

$$k = \frac{1 + \alpha}{1 - \alpha}$$

We calculated these functions in the table 9 by the recurrence relations (13) for the 9 values of the α parameter and for j up to 20.

Finally, in the intermediate temperature expansion we were lead to compute the $\zeta_{10}(2n)$ defined by (9). The values are given in table 10 with 6 significant figures for n varying from 1 to 19.

CONCLUSIONS

Our complete results confirm the definite disagreement with BLACKMAN'S numerical integration already found in (B). The inflexion point of the specific heat curve, missing in BLACKMAN'S work, remains for all value of the mass ration. Moreover, at low temperature our curves do not coincide with BLACKMAN'S ones. This is particularly appearent in the effective DEBYE temperature curves (fig. 4) where for high values of the α parameter we obtain a minimum while for low values of α our minimum is more pronounced than BLACKMAN'S one.

This work leads us to meet a new class of transcendant functions $\sigma(\alpha, \tau)$ which are a generalization of the $\sigma(\tau)$ found by J. PIRENNE and P. RENSON in their study of the monoatomic chain. These functions do not seem to have been studied. We gave here extensive numerical tables of them, diagrams and various expansions in powers of τ. But it seems that a more complete analytical treatment should be interesting for they provide a very useful tool for the study of the disordered diatomic chain.

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TABLE I

τ \ α	0	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9
0	1	0,99906	0,99618	0,99127	0,98412	0,97437	0,96149	0,94439	0,92110	0,88641
0,10	0,82680	0,82592	0,82347	0,81921	0,81302	0,80463	0,79365	0,77927	0,76012	0,73292
0,25	0,67840	0,67775	0,67576	0,67238	0,66751	0,66097	0,65252	0,64174	0,62792	0,60972
0,50	0,51961	0,51918	0,51788	0,51572	0,51263	0,50855	0,50342	0,49710	0,48944	0,48020
0,75	0,41545	0,41518	0,41439	0,41306	0,41117	0,40872	0,40567	0,40200	0,39767	0,39263
1,00	0,34253	0,34236	0,34187	0,34104	0,33988	0,33838	0,33654	0,33433	0,33176	0,32881
1,50	0,24954	0,24947	0,24926	0,24891	0,24843	0,24780	0,24703	0,24612	0,24506	0,24386
2,00	0,19436	0,19433	0,19423	0,19406	0,19382	0,19351	0,19314	0,19269	0,19218	0,19160
2,50	0,15849	0,15847	0,15842	0,15832	0,15819	0,15802	0,15782	0,15757	0,15729	0,15697
3,00	0,13352	0,13351	0,13348	0,13342	0,13334	0,13324	0,13312	0,13297	0,13280	0,13261
4,00	0,10127	0,10127	0,10125	0,10123	0,10119	0,10115	0,10109	0,10103	0,10095	0,10087
5,00	0,08145	0,08145	0,08144	0,08143	0,08141	0,08139	0,08136	0,08132	0,08128	0,08124
∞	0,00000	0,00000	0,00000	0,00000	000,000	0,00000	0,00000	0,00000	0,00000	0,00000

Numerical values of the $\sigma(\alpha, \tau)$*function*

TABLE 2

τ \ α	0	0,1	0,2	0,2	0,4	0,5	0,6	0,7	0,8	0,9
0,00	1	0,99906	0,99618	0,99127	0,98412	0,97437	0,96149	0,94439	0,92110	0,88641
0,10	0,95083	0,94984	0,94704	0,94214	0,93503	0,92533	0,91252	0,89554	0,87247	0,83828
0,25	0,88023	0,87931	0,87652	0,87177	0,86485	0,85546	0,84308	0,82684	0,80511	0,77428
0,50	0,77113	0,77030	0,76782	0,76359	0,75751	0,74937	0,73888	0,72561	0,70891	0,68775
0,75	0,67359	0,67294	0,67098	0,66768	0,66299	0,65681	0,64905	0,63955	0,62811	0,61446
1,00	0,58899	0,58852	0,58711	0,58474	0,58139	0,57703	0,57163	0,56513	0,55747	0,54857
1,50	0,45841	0,45819	0,45748	0,45631	0,45467	0,45257	0,44996	0,44687	0,44329	0,43920
2,00	0,36868	0,36856	0,36819	0,36758	0,36672	0,36562	0,36426	0,36266	0,36081	0,35870
2,50	0,30587	0,30580	0,30559	0,30524	0,30475	0,30412	0,30335	0,30244	0,30139	0,30019
3,00	0,26032	0,26027	0,26015	0,25993	0,25963	0,25924	0,25876	0,25820	0,25756	0,25682
4,00	0,19957	0,19955	0,19949	0,19940	0,19926	0,19908	0,19887	0,19862	0,19833	0,19800
5,00	0,16135	0,16133	0,16130	0,16125	0,16118	0,16109	0,16098	0,16084	0,16069	0,16052
∞	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000

Numerical values of the $\sigma^1/_2(\alpha, \tau)$ *function*

TABLE 3

τ \ α	0,	0,1	0,2	0,3	0,4	0,5	0,6	9,7	0,8	0,9
0,00	1	0,99906	0,99618	0,99127	0,98412	0,97437	0,96149	0,94439	0,92110	0,88641
0,10	0,99917	0,99818	0,99534	0,99041	0,98323	0,97342	0,96046	0,94324	0,91974	0,88455
0,25	0,99474	0,99376	0,99080	0,98574	0,97834	0,96833	0,95472	0,93655	0,91148	0,87227
0,50	0,97821	0,97710	0,97374	0,96797	0,95950	0,94784	0,93224	0,91142	0,88324	0,84380
0,75	0,94737	0,94615	0,94246	0,93619	0,92712	0,91494	0,89918	0,87920	0,85410	0,82256
1,00	0,90053	0,89940	0,89602	0,89032	0,88220	0,87151	0,85804	0,84153	0,82164	0,79792
1,50	0,78121	0,78050	0,77836	0,77478	0,76974	0,76322	0,75518	0,74556	0,73432	0,72140
2,00	0,66575	0,66534	0,66409	0,66200	0,65907	0,65530	0,65067	0,64518	0,63881	0,63156
2,50	0,57055	0,57030	0,56954	0,56829	0,56652	0,56425	0,56147	0,55818	0,55438	0,55005
3,00	0,49514	0,49498	0,49450	0,49370	0,49258	0,49114	0,48937	0,48729	0,48488	0,48215
4,00	0,38760	0,38753	0,38731	0,38694	0,38641	0,38575	0,38493	0,38396	0,38284	0,38158
5,00	0,31658	0,31654	0,31642	0,31622	0,31595	0,31559	0,31515	0,31463	0,31403	0,31335
∞	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000	0,00000

Numerical values of the $\sigma^{3/2}(\alpha, \tau)$ *function*

TABLE 4

t \ α	0	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9
0	1	0,999	0,996	0,991	0,984	0,974	0,961	0,944	0,921	0,886
0,050	0,999	0,998	0,995	0,990	0,983	0,973	0,960	0,943	0,920	0,885
0,125	0,995	0,994	0,991	0,986	0,978	0,968	0,955	0,937	0,912	0,874
0,250	0,979	0,978	0,975	0,969	0,961	0,950	0,935	0,915	0,885	0,836
0,375	0,953	0,952	0,948	0,941	0,932	0,919	0,901	0,876	0,839	0,774
0,500	0,915	0,914	0,909	0,902	0,891	0,875	0,853	0,823	0,777	0,694
0,750	0,804	0,802	0,796	0,786	0,770	0,749	0,718	0,675	0,608	0,487
1	0,646	0,644	0,636	0,622	0,602	0,573	0,533	0,476	0,389	0,228
1,25	0,444	0,441	0,432	0,415	0,390	0,354	0,304	0,233	0,124	—0,076
1,50	0,203	0,199	0,188	0,168	0,138	0,095	0,035	—0,050	—0,181	—0,421
2	—0,382	—0,386	—0,402	—0,429	—0,469	—0,525	—0,605	—0,718	—0,893	—1,212
2,50	—1,080	—1,086	—1,105	—1,139	—1,189	—1,259	—1,359	—1,501	—1,718	—2,118
∞	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$

Numerical values of the $\mathcal{F}(\alpha, t)$ function

TABLE 5

t \ α	0	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9
0	1,000	1,000	0,996	0,991	0,984	0,974	0,961	0,944	0,921	0,886
0,050	1,000	1,000	0,997	0,992	0,985	0,975	0,963	0,946	0,922	0,888
0,125	1,005	1,004	1,002	0,997	0,990	0,980	0,968	0,952	0,930	0,899
0,250	1,021	1,020	1,018	1,014	1,008	0,999	0,989	0,976	0,959	0,938
0,375	1,049	1,048	1,046	1,043	1,038	1,032	1,024	1,015	1,003	0,989
0,5	1,089	1,089	1,087	1,085	1,081	1,077	1,072	1,065	1,057	1,049
0,75	1,208	1,208	1,207	1,206	1,205	1,203	1,200	1,197	1,193	1,189
1	1,369	1,369	1,368	1,368	1,367	1,366	1,364	1,363	1,361	1,359
1,25	1,556	1,556	1,556	1,555	1,555	1,554	1,553	1,552	1,551	1,550
1,50	1,760	1,760	1,760	1,760	1,760	1,759	1,759	1,758	1,758	1,757
2	2,200	2,200	2,199	2,199	2,199	2,1999	2,1999	2,199	2,198	2,198
2,50	2,662	2,661	2,661	2,661	2,661	2,661	2,661	2,661	2,661	2,661
∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

Numerical values of the $\xi(\alpha, t)$ function

TABLE 6

t \ α	0	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9
0	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
0,05	0,033	0,033	0,034	0,035	0,036	0,038	0,041	0,046	0,055	0,075
0,125	0,084	0,084	0,085	0,087	0,091	0,096	0,105	0,118	0,142	0,200
0,250	0,168	0,169	0,172	0,177	0,185	0,197	0,215	0,244	0,295	0,407
0,375	0,256	0,257	0,262	0,270	0,282	0,301	0,328	0,369	0,437	0,574
0,50	0,348	0,350	0,356	0,366	0,382	0,404	0,437	0,485	0,562	0,710
0,75	0,539	0,541	0,548	0,561	0,579	0,605	0,643	0,697	0,780	0,936
1	0,723	0,726	0,732	0,745	0,765	0,792	0,831	0,886	0,972	1,131
1,25	0,890	0,892	0,899	0,912	0,932	0,956	0,999	1,056	1,142	1,301
1,50	1,038	1,041	1,048	1,062	1,081	1,110	1,149	1,205	1,292	1,452
2	1,291	1,293	1,301	1,314	1,334	1,362	1,402	1,458	1,545	1,705
2,50	1,497	1,499	1,507	1,520	1,540	1,568	1,608	1,665	1,752	1,911
∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

Numerical values of the $\mathscr{P}(\alpha, t)$ function

TABLE 7

t \ α	0	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9
0	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
0,05	0,033	0,033	0,034	0,035	0,036	0,038	0,041	0,046	0,055	0,075
0,125	0,084	0,084	0,086	0,088	0,092	0,098	0,107	0,122	0,149	0,216
0,250	0,172	0,173	0,176	0,182	0,192	0,206	0,227	0,257	0,303	0,376
0,375	0,270	0,271	0,276	0,284	0,296	0,312	0,333	0,361	0,397	0,445
0,50	0,376	0,378	0,382	0,389	0,398	0,411	0,427	0,447	0,472	0,501
0,75	0,570	0,570	0,572	0,575	0,580	0,586	0,593	0,602	0,612	0,624
1	0,703	0,703	0,704	0,706	0,708	0,710	0,714	0,717	0,722	0,727
1,25	0,788	0,788	0,789	0,790	0,791	0,792	0,794	0,795	0,798	0,800
1,50	0,844	0,844	0,844	0,844	0,845	0,845	0,846	0,847	0,848	0,850
2	0,906	0,906	0,906	0,906	0,906	0,907	0,907	0,907	0,908	0,908
2,50	0,938	0,938	0,938	0,938	0,938	0,938	0,938	0,938	0,939	0,939
∞	1,000	1,000	1,000	1,000	1,000	1,000	1,000	1,000	1,000	1,000

Numerical values of the $\mathscr{C}(\alpha, t)$ function

TABLE 8

α	$\varkappa(\alpha)$
0	— 1,08879
0,1	— 1,09239
0,2	— 1,10443
0,3	— 1,12541
0,4	— 1,15683
0,5	— 1,20133
0,6	— 1,26362
0,7	— 1,35282
0,8	— 1,48966
0,9	— 1,74072

Numerical values of the $\varkappa(\alpha)$ *function*

TABLE 9

J \ α	0,1	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9
0	20,3264	18,0971	17,0810	16,5152	16,1742	15,9627	15,8326	15,7571	15,7189
1	14,4829	13,7609	13,6456	13,7554	13,9776	14,2646	14,5922	14,9471	15,3207
2	10,7983	10,8123	11,1570	11,6401	12,2047	12,8264	13,4933	14,1984	14,9376
3	08,4214	08,7726	09,3321	10,0053	10,7659	11,6047	12,5183	13,5059	14,5688
4	06,8474	07,3341	07,9754	08,7300	09,5916	10,5632	11,6516	12,8650	14,2137
5	05,7740	06,2980	06,9521	07,7255	08,6272	09,6722	10,8798	12,2713	13,8719
6	05,0185	05,5348	06,1680	06,9261	07,8299	08,9070	10,1911	11,7209	13,5428
7	04,4691	04,9593	05,5574	06,2829	07,1663	08,2473	09,5754	11,2104	13,2257
8	04,0563	04,5150	05,0740	05,7596	06,6101	07,6763	08,0289	10,7363	12,9203
9	03,7366	04,1642	04,6848	05,3290	06,1406	07,1799	08,5288	10,2957	12,6261
10	03,4817	03,8809	04,3664	04,9706	05,7412	06,7466	08,0833	09,8860	12,3423
11	03,2733	03,6476	04,1018	04,6690	05,3991	06,3667	07,6817	09,5046	12,0692
12	03,0992	03,4519	03,8787	04,4123	05,1038	06,0321	07,3188	09,1493	11,8057
13	02,9509	03,2850	03,6879	04,1916	04,8471	05,7361	06,9902	08,8180	11,5516
14	02,8227	03,1406	03,5228	03,9999	04,6222	05,4732	06,6918	08,5088	11,3066
15	02,7103	03,0142	03,3783	03,8319	04,4240	05,2385	064,204	08,2200	11,0703
16	02,6107	02,9022	03,2504	03,6833	04,2480	05,0281	06,1728	07,9499	10,8423
17	02,5216	02,8022	03,1364	03,5508	04,0908	04,8388	05,9466	07,6972	10,6223
18	02,4411	02,7120	03,0339	03,4318	03,9495	04,6676	05,7392	07,4604	10,4099
19	02,3681	02,6302	02,9409	03,3242	03,8218	04,5122	05,5487	07,2384	10,2049
20	02,3013	02,5555	02,8563	03,2263	03,7057	04,3705	05,3734	07,0301	10,0070

Numerical values of the V_j *functions*

TABLE 10

n	$\zeta_{10}(2n)$
1	$9{,}51663\ 10^{-2}$
2	$2{,}86650\ 10^{-4}$
3	$1{,}54954\ 10^{-6}$
4	$9{,}94268\ 10^{-9}$
5	$6{,}92686\ 10^{-11}$
6	$5{,}06219\ 10^{-13}$
7	$3{,}81542\ 10^{-15}$
8	$2{,}93753\ 10^{-17}$
9	$2{,}29656\ 10^{-19}$
10	$1{,}81605\ 10^{-21}$
11	$1{,}44861\ 10^{-23}$
12	$1.16334\ 10^{-25}$
13	$9{,}39225\ 10^{-28}$
14	$7{,}61498\ 10^{-30}$
15	$6.19504\ 10^{-32}$
16	$5.05375\ 10^{-34}$
17	$4.13197\ 10^{-36}$
18	$3.38451\ 10^{-38}$
19	$2.77644\ 10^{-40}$

Numerical values of the incomplete Riemanian function $\zeta_{10}(2n)$