

Moment Singularity Expansion for the Density of States*

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A systematic approximation procedure is developed to determine the density of states associated with a particular energy band. The density of states is expressed as the sum of two functions, one of which contains the discontinuous derivatives produced by critical points, and is determined once the effective masses at these points are known; the other is smooth, and is expanded in Jacobi polynomials. The coefficients in this expansion are determined from the moments of the distribution. Two applications of the method are given.

THE calculation of the density of states has been a central problem in the theory of lattice vibrations, and in energy band theory for many years. As a result of the work of Van Hove¹ and Phillips^{2,3} the fundamental analytic properties of the density of states (DS)—in particular, the nature of the singularities—are well understood. It remains a formidable problem to compute this function accurately for a particular system.

One approach to the determination of the DS is that of numerical sampling: The energy (or frequency) is numerically evaluated at a sufficiently large number of points in the Brillouin zone to allow an estimate of the portion of the volume of the zone in which the states have energies in a certain range. There are two principal disadvantages to this procedure: first, the method is quite laborious, since a large number of points must be considered; and second, the DS itself is not obtained, instead an average of the DS over some finite energy range is determined. The latter difficulty is a serious one, since the function is known to have singularities at which the first derivative has an infinite discontinuity. A second, frequently used procedure is the method of moments, which was first introduced by Montroll.^{4,5} In this method, one expands the DS in terms of some convenient set of polynomials. The coefficients are determined from the moments of the DS, which can usually be computed independently. One still has the difficulty in this method that any approximating polynomial will have derivatives of all orders, and hence the required behavior at critical points will not be reproduced. Further, the existence of singular derivatives in the DS implies that the moment expansion will converge rather slowly.

A method of alleviating this difficulty of the moment expansion was proposed by Lax and Lebowitz.⁶ The density of states, $N(E)$, is expressed as the sum of two functions, $G(E)$ and $H(E)$, where $G(E)$ is a specified function with the discontinuous derivatives produced

by critical points in the $E(k)$ relation. The parameters of this function can be determined from the effective masses at critical points. The function $H(E)$ is smooth, and can easily be approximated by a polynomial. In this paper, the work of Lax and Lebowitz has been extended in several respects; particularly in regard to the choice of the singular function, and in the selection of the set of polynomials in which $H(E)$ is expanded. Jacobi polynomials, rather than Legendre polynomials, have been chosen because of the particular orthogonality properties of these functions. In addition, Lax and Lebowitz applied their approach only to the distribution function of the vibration frequencies of a two-dimensional square lattice. Applications to three-dimensional systems are considered here.

First, we review the analytic properties of the DS. The DS is defined so that $N(E)dE$ is the number of states per unit volume with energies between E and $E+dE$. It may be expressed as

$$N(E) = \frac{2}{8\pi^3} \frac{d}{dE} \int d^3k = \frac{1}{4\pi^3} \int \frac{dS_E}{|\nabla_{\mathbf{k}}E|} \quad (1)$$

in which the first integral includes all \mathbf{k} space enclosed by a surface of constant energy E , and the integral in the second expression covers a surface of constant energy. For simplicity, we consider bands which have only analytic critical points (in the sense of Van Hove¹ and Phillips²). (An analytic critical point is a point in \mathbf{k} space where the gradient of the energy vanishes, and an expansion of the energy in powers of k is possible.) "S" bands in cubic lattices are examples of such bands.

Consider the energy near a minimum of the band. The energy then possesses an expansion in powers of the wave vector which, in the case of a cubic lattice, may be written as

$$E(\mathbf{k}) = \sum_n k^{2n} [E_{2n} + \sum_{l \leq 2n} E_{2n,l} \mathcal{K}_l(\theta, \phi)] \quad (2)$$

in which $\mathcal{K}_l(\theta, \phi)$ is a "Kubic harmonic" belonging to the completely symmetric representation.⁷ It is a linear combination of spherical harmonics of l th order. To compute $N(E)$ in this case, it is convenient to use, in-

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¹ L. Van Hove, Phys. Rev. **89**, 1189 (1953).

² J. C. Phillips, Phys. Rev. **104**, 1263 (1956).

³ J. C. Phillips and H. B. Rosenstock, J. Phys. Chem. Solids **5**, 288 (1958).

⁴ E. W. Montroll, J. Chem. Phys. **10**, 218 (1942).

⁵ E. W. Montroll, J. Chem. Phys. **11**, 481 (1943).

⁶ M. Lax and J. L. Lebowitz, Phys. Rev. **96**, 594 (1954).

⁷ F. C. von der Lage and H. A. Bethe, Phys. Rev. **71**, 612 (1957).

stead of Eq. (1), the equivalent expression⁸:

$$N(E) = \frac{1}{12\pi^3} \frac{d}{dE} \int k^3(E, \theta, \phi) \sin\theta d\theta d\phi. \quad (3)$$

Equation (2) can be solved by iteration to give k^2 as a function of energy and angle. The integration over solid angle can be accomplished using the orthonormality relations for the Kubic harmonics. The DS can then be written formally as

$$N(E) = (E - E_0)^{1/2} \sum_n \alpha_n (E - E_0)^n. \quad (4)$$

The DS can evidently be expressed as a series in odd half integral powers of the energy. The coefficients α_n are fairly complicated combinations of the E_{2n} and $E_{2n,i}$ so that usually it is practical to compute only a few of them. The first three are given below:

$$\begin{aligned} \alpha_0 &= 1/2\pi^2 E_2^{3/2}, \\ \alpha_1 &= -5E_4/4\pi^2 E_2^{7/2}, \\ \alpha_2 &= -(7/4\pi^2 E_2^{9/2}) [E_6 - (9/4E_2)(E_4^2 + E_{4,4}^2)]. \end{aligned} \quad (5)$$

The series presumably converges for energies less than that of the first saddle point. An analysis similar to that leading to Eq. (4) can also be made near a maximum. The result is formally similar to (4), except that the independent variable is $E_m - E$ (where E_m is the energy of the maximum), rather than $E - E_0$.

The behavior of the DS near a saddle point of the band structure has been analyzed previously.^{1,2} The simplest discussion seems to be that of Wannier.⁹ If E_s is the energy of the saddle point, the DS contains a term of the form $(E_s - E)^{1/2}$ or $(E - E_s)^{1/2}$. The derivative of the DS has an infinite discontinuity for $E = E_s$. The singular term is superimposed on a smooth background function. There are two types of saddle points. In one case we have

$$E(\mathbf{k}) - E_s = \alpha k_1^2 + \beta k_2^2 - \gamma k_3^2 + O(k^4), \quad (6)$$

in which α, β, γ are positive, and $k_1, k_2,$ and k_3 are measured along the principal axes. The part of $N(E)$ which has the singular derivatives is

$$\begin{aligned} & -(E_s - E)^{1/2} / 4\pi^2 (\alpha\beta\gamma)^{1/2} \quad \text{for } E \leq E_s, \\ & 0 \quad \text{for } E \geq E_s. \end{aligned} \quad (7)$$

Similarly, if

$$E(\mathbf{k}) - E_s = \alpha' k_1^2 - \beta' k_2^2 - \gamma' k_3^2, \quad (8)$$

the singular part is

$$\begin{aligned} & 0 \quad \text{for } E \leq E_s, \\ & -(E - E_s)^{1/2} / 4\pi^2 (\alpha'\beta'\gamma')^{1/2} \quad \text{for } E \geq E_s. \end{aligned} \quad (9)$$

Except for the singular parts just described, the density of states is a smooth function of energy. Let

⁸ J. de Launay, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1956), Vol. 2, p. 219.
⁹ G. H. Wannier, *Elements of Solid State Theory* (Cambridge University Press, New York, 1959), p. 70.

E_m and E_0 be the energies of states at the top and bottom of the band. It is convenient to define a new variable z by

$$z^2 = (E - E_0) / (E_m - E_0). \quad (10)$$

We write $n(z)$ to designate the DS with the energy variable replaced by z according to (10). The function $n(z)$ is expressed as

$$n(z) = g(z) + h(z), \quad (11)$$

in which $g(z)$ is a function with singular derivatives as previously described, and which will be specified below; and $h(z)$ is a smooth function with vanishing first derivatives at the top and bottom of the band.

For simplicity, we consider a simple band with one maximum, one minimum (both assumed to be spherical), and \mathfrak{N} saddle points of each kind. The generalization to more complicated bands is straightforward. Let the saddle points of the type specified by Eq. (6) occur for $z = z_1$ and those specified by (8) for $z = z_2$. We denote by E_2' the reciprocal effective mass at the top of the band. A suitable choice for $g(z)$ is as follows:

$$\begin{aligned} g(z) &= \frac{(E_m - E_0)^{1/2}}{2\pi^2} \left[\frac{z(1-z^2)^{3/2}}{E_2^{3/2}} + \frac{z^3(1-z^2)^{1/2}}{(E_2')^{3/2}} \right. \\ &\quad - \frac{\mathfrak{N}}{2(\alpha\beta\gamma)^{1/2}} \left(\frac{z}{z_1} \right)^3 (z_1^2 - z^2)^{1/2} \eta(z_1 - z) \\ &\quad \left. - \frac{\mathfrak{N}}{2(\alpha'\beta'\gamma')^{1/2}} \frac{(1-z^2)^{3/2}}{(1-z_2^2)^{3/2}} (z^2 - z_2^2)^{1/2} \eta(z - z_2) \right], \quad (12) \end{aligned}$$

where η is the unit step function, which has the property that

$$\begin{aligned} \eta(x) &= 0 \quad \text{for } x < 0, \\ \eta(x) &= 1 \quad \text{for } x > 0. \end{aligned}$$

The function $g(z)$ has been constructed to have the characteristic behavior of the DS at each critical point. The complete DS, $n(z)$, differs from $g(z)$ by terms of the order z^3 near $z=0$, and by terms of order $(1-z^2)^{3/2}$ near $z=1$. It is desirable to include this property explicitly in the expression for $h(z)$. To do this we write

$$h(z) = z^3 (1-z^2)^{3/2} h'(z). \quad (13)$$

The function $h'(z)$ which is defined by (13) is of order unity at $z=0$ and $z=1$. It is to be expanded in a set of orthogonal polynomials. The choice of polynomials for the expansion is determined by two requirements: The polynomials must be orthogonal with respect to a weight function consistent with (13); and second, it must be possible to evaluate integrals containing the DS and a polynomial independently of the expression (11) for $n(z)$.

A particular set of Jacobi polynomials possess the required properties. The function $h'(z)$ is expressed as

$$h'(z) = \sum_n c_n P_n^{(\alpha, \beta)}(1-2z^2), \quad (14)$$

TABLE I. Coefficients of Jacobi polynomials appearing in the expansion of the smooth part of the density of states for the energy band specified by Eq. (26). The coefficients of the polynomials with odd n vanish.

n	c_n	n	c_n
0	1.5977618	6	0.0736
2	-0.13966731	8	-0.089
4	-0.0161960		

in which the notation for the Jacobi polynomial is that of Erdelyi *et al.*,¹⁰ and α and β are for the moment undetermined. Now multiply both sides of (11) by $zP_l^{(\alpha,\beta)}(1-2z^2)$ and integrate on z :

$$\int_0^1 n(z)P_l^{(\alpha,\beta)}(1-2z^2)zdz = \int_0^1 g(z)P_l^{(\alpha,\beta)}(1-2z^2)zdz + \sum_n c_n \int_0^1 P_n^{(\alpha,\beta)}(1-2z^2)P_l^{(\alpha,\beta)}(1-2z^2)z^4(1-z^2)^{3/2}dz.$$

The Jacobi polynomials obey the orthogonality relation

$$\int_{-1}^1 P_l^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(x)(1-x)^\alpha(1+x)^\beta dx = h_n \delta_{ln} \quad (15)$$

in which

$$h_n = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\Gamma(n+\alpha+\beta+1)}. \quad (16)$$

The substitution $x=1-2z^2$ makes this relation useful for our purposes provided that we also choose $\alpha=\beta=3/2$. The coefficients c_n are now determined to be

$$c_n = \frac{32}{h_n} \left[\int_0^1 n(z)P_n^{(3/2,3/2)}(1-2z^2)zdz - \int_0^1 g(z)P_n^{(3/2,3/2)}(1-2z^2)zdz \right]. \quad (17)$$

The Jacobi polynomials are expressed as

$$P_n^{(3/2,3/2)}(1-2z^2) = \sum_{j=0}^n a_j^{(n)} z^{2j}. \quad (18)$$

The coefficients a_j are given by

$$a_j^{(n)} = \sum_{m=0}^n \binom{n+3/2}{m} \binom{n+3/2}{n-m} \binom{m}{m+j-n}. \quad (19)$$

The following recurrence relation is also useful:

$$P_{n+1}^{(3/2,3/2)}(x) = \frac{2n+5}{(n+1)(n+4)} [(n+2)xP_n^{(3/2,3/2)}(x) - \frac{1}{2}(n+3/2)P_{n-1}^{(3/2,3/2)}(x)]. \quad (20)$$

¹⁰ A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw Hill Book Company, Inc., New York, 1953), Vol. 2, p. 168.

The first seven polynomials are given explicitly below:

$$\begin{aligned} P_0^{(3/2,3/2)}(x) &= 1, \\ P_1^{(3/2,3/2)}(x) &= (5/2)x, \\ P_2^{(3/2,3/2)}(x) &= (7/8)(6x^2-1), \\ P_3^{(3/2,3/2)}(x) &= (21/2)[x^3-(3/8)x], \\ P_4^{(3/2,3/2)}(x) &= (33/8)(5x^4-3x^2+3/16), \\ P_5^{(3/2,3/2)}(x) &= (429/64)[6x^5-5x^3+(3/4)x], \\ P_6^{(3/2,3/2)}(x) &= (715/128)[14x^6-15x^4+(15/4)x^2-1/8]. \end{aligned} \quad (21)$$

Equation (17) is useful because it is possible to determine the integrals

$$\int_0^1 P_n^{(3/2,3/2)}(1-2z^2)n(z)zdz$$

independently. The n th moment of the DS is defined by

$$\begin{aligned} M_n &= \int_{E_0}^{E_m} N(E)(E-E_0)^n dE \\ &= 2(E_m-E_0)^{n+1} \int_0^1 z^{2n+1}n(z)dz. \end{aligned} \quad (22)$$

It follows from Eq. (1) that these may also be expressed as

$$M_n = \frac{2}{(8\pi^3)} \int [E(\mathbf{k})-E_0]^n d^3k. \quad (23)$$

Evidently, the M_n can be determined if $E(k)$ is known. The matrix techniques which are used to compute moments in the theory of lattice vibrations are not usually available in energy band theory, except when the tight-binding approximation is employed.

The moments M_n' of the singular function $g(z)$, which are defined by

$$M_n' = \int_0^1 g(z)z^{2n+1}dz, \quad (24)$$

can be computed by elementary techniques. Explicit expressions are given in the Appendix. One then has finally

$$c_n = \frac{32}{h_n} \sum_i a_i^{(n)} \left[\frac{M_j}{2(E_m-E_0)^{j+1}} - M_j' \right]. \quad (25)$$

At each stage of approximation, the density of states which is computed from (11) has the correct analytic properties. One can expect that the convergence of the expansion (14) will be sufficiently rapid so that only a relatively small number of terms need be included.

In order to illustrate the application of the procedure developed here, we have considered two examples. The first of these is the calculation of the DS pertaining to the band

$$E(\mathbf{k}) = 3 - (\cos k_x + \cos k_y + \cos k_z), \quad (26)$$

for which an exact result has been given by Bowers and Rosenstock¹¹ and by Montroll.¹² In this case it is possible to obtain a general expression for the moments M_j which yields, in combination with Eqs. (19), (24), and (25), a complete solution to the problem of computing the DS by the moment singularity method. The computation of the moments is accomplished as follows: The j th moment M_j may be expressed as a combination of "small" moments m_i :

$$M_j = 2 \sum_i (3)^{i-i} (-1)^i \binom{j}{i} m_i, \quad (27)$$

where the $\binom{j}{i}$ are binomial coefficients and

$$m_i = (2\pi)^{-3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} (\cos k_x + \cos k_y + \cos k_z)^i dk_x dk_y dk_z.$$

The small moments may be computed through a trinomial expansion,

$$\begin{aligned} m_i &= (2\pi)^{-3} \sum_r \sum_s \binom{i}{r} \binom{i-r}{s} \\ &\times \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \cos^r k_x \cos^s k_y \cos^{i-r-s} k_z dk_x dk_y dk_z \\ &= - \sum_{i/2}^i \sum_{p=0}^{i/2} \sum_{t=0}^p [t!(p-t)!(\frac{1}{2}i-p)!]^{-2} \text{ if } i \text{ is even} \\ &= 0 \text{ if } i \text{ is odd.} \end{aligned} \quad (28)$$

Since the moments of the singular function are elementary integrals, and the coefficients $a_j^{(n)}$ have been given, the coefficients c_n of the Jacobi polynomials in the expansion of the DS are determined for arbitrary n . The formal result is, however, quite lengthy, and need not be given here. The values of the first five nonzero coefficients c_n have been computed, and are given in Table I. The DS which is determined from them is shown in Fig. 1, where it is compared with the exact result. The agreement is quite good.

It is useful to compare the moment-singularity expansion of the DS with conventional methods in which the singularities of the DS are not explicitly designated. Earlier calculations with the method of moments have generally employed the Legendre polynomials as the basic set of functions. An expansion, which is no more complicated than that using the Legendre polynomials, but which makes use of more detailed information concerning the analytic properties of the DS has been proposed by Sack.¹³ It makes use of the Tchebicheff

¹¹ W. Bowers and H. B. Rosenstock, *J. Chem. Phys.* **18**, 1056 (1950).

¹² E. W. Montroll, in *Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability* (University of California Press, Berkeley, California, 1956), Vol. 3, p. 209.

¹³ R. A. Sack, *Bull. Am. Phys. Soc.* **6**, 293 (1961).

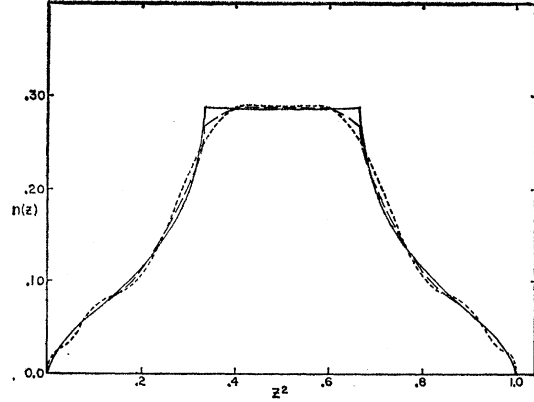


FIG. 1. Density of states for the energy band of Eq. (26). The solid curve is the exact result of Bowers and Rosenstock (reference 11) and Montroll (reference 12), the long dashes show the result of the moment singularity expansion (11) including the first five Jacobi polynomials with nonzero coefficients; the curve composed of short dashes shows the result of the moment expansion (30) including the first six Tchebicheff polynomials with nonzero coefficients.

polynomials of the second kind, $U_n(z)$. These functions satisfy the orthogonality relation:

$$\int_{-1}^1 U_n(z) U_l(z) (1-z^2)^{1/2} dz = \frac{1}{2} \pi \delta_{nl}. \quad (29)$$

If the index n is odd, only odd powers of z are present in $U_n(z)$. The expansion is the following:

$$n(z) = (1-z^2)^{1/2} \sum_{n \text{ odd}} b_n U_n(z). \quad (30)$$

The multiplying function $(1-z^2)^{1/2}$ ensures that the DS has the proper behavior at the top of the band, the restriction to odd powers of z insures the same thing at the bottom of the band. The effects of saddle points are not explicitly included. The coefficients b_n are found to be

$$b_n = - \frac{4}{\pi} \int_0^1 n(z) U_n(z) dz. \quad (31)$$

The b_n may be expressed in terms of the moments. A Tchebicheff polynomial is expressed in powers of z :

$$U_n(z) = \sum_j d_j^{(n)} z^{2j+1}. \quad (32)$$

The coefficients $d_j^{(n)}$ are given by

$$\begin{aligned} d_j^{(n)} &= 2^{j+1} (-1)^{(n-1-2j)/2} \left(\frac{n+2j+1}{2} \right)! \\ &\times \left[(2j+1)! \left(\frac{n-2j-1}{2} \right)! \right]^{-1}. \end{aligned} \quad (33)$$

Equation (22) enables us to express b_n as

$$b_n = (2/\pi) \sum d_j^{(n)} [M_j / (E_m - E_0)^{j+1}]. \quad (34)$$

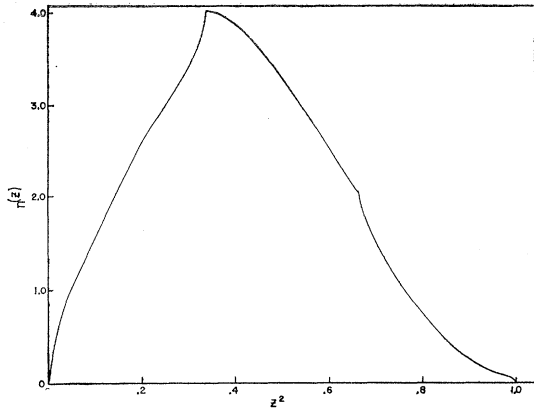


FIG. 2. Density of states for the energy band of the Mathieu problem, obtained from Eq. (11) including the first five Jacobi polynomials.

If the moments M_j can be calculated, one has in principle a solution to the problem of calculating the DS. For the reasons discussed in the beginning of the paper, one does not expect to obtain as good a representation of the DS with a small number of Tchebicheff polynomials as is possible with an appropriate singular function and a small number of Jacobi polynomials. Nevertheless, this procedure may be useful, particularly in cases in which it is not feasible to locate all the critical points of the DS.

The procedure of expansion in Tchebicheff polynomials has been applied to the simple band of Eq. (26). The first six coefficients are listed in Table II, and the DS which is computed from them is shown in Fig. 1. Although one more polynomial is present here than in the previous case, the fit to the exact density of states is noticeably poorer. The gain in accuracy resulting from inclusion of an appropriate singular function is quite evident.

As a second example of the application of the moment singularity method, the DS has been computed for the lowest energy band which is the solution of the Schrödinger equation for the potential

$$V = 2V_0[\cos(2\pi x/a) + \cos(2\pi y/a) + \cos(2\pi z/a)]. \quad (35)$$

This is the Mathieu problem, which has previously been discussed by Slater.¹⁴ The details of the band calculation in this problem will be discussed elsewhere. For the purpose of computing the moments, the energy was expressed as a Fourier series, and the coefficients of the first eleven terms were found. The numerical accuracy of the band calculation is sufficient for the effective masses to be determined by differentiation of the series. In Fig. 2, the DS is shown for the case $(ma^2V_0/2\pi^2\hbar^2) = 0.1$. The first five Jacobi polynomials were included in the calculation.

The principal problem which is encountered in the actual calculation of the DS by the moment singularity

¹⁴ J. C. Slater, Phys. Rev. **87**, 807 (1952).

TABLE II. Coefficients of Tchebicheff polynomials appearing in the expansion of the density of states for the energy specified by Eq. (26). Only polynomials with n odd appear in the expansion; the coefficients of alternate odd polynomials ($n=3, 7, 11, 15, 19$, etc.) vanish.

n	b_n	n	b_n
1	0.21220659	13	-0.0008733
5	-0.07073553	17	-0.009024
9	0.02357851	21	0.010770

expansion is that of retaining sufficient numerical accuracy in the calculations of the moments to obtain significant results for the coefficients c_n . There is a very substantial amount of cancellation in the computation of the c_n : seven-figure accuracy in the moments yields only two significant figures in the determination of c_8 for the first problem discussed. The problem of numerical accuracy was noticed by Montroll in his original work on the method of moments,⁵ and appears to be common to all moment expansions for the DS.

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APPENDIX

In this Appendix, we give expressions for the moments of the singular function, M_n' which are defined in Eq. (24) of the text. The singular function $g(z)$ is given in Eq. (12). The results are

$$M_n' = \frac{(E_m - E_0)^{1/2}}{2\pi^2} [(E_2)^{-3/2} g_1(n) + (E_2')^{-3/2} g_2(n) - \frac{1}{2} \mathfrak{U}(\alpha\beta\gamma)^{-1/2} g_3(n) - \frac{1}{2} \mathfrak{U}(\alpha'\beta'\gamma')^{-1/2} g_4(n)]. \quad (A1)$$

The integrals g_1 , etc., are given by

$$g_1(n) = \int_0^1 z^{2n+2} (1-z^2)^{3/2} dz = \frac{3\pi}{2} \frac{1 \times 3 \times 5 \times \cdots \times (2n+1)}{2 \times 4 \times 6 \times \cdots \times (2n+6)}, \quad (A2)$$

$$g_2(n) = \int_0^1 z^{2n+4} (1-z^2)^{1/2} dz = \frac{2n+3}{3} g_1(n), \quad (A3)$$

$$g_3(n) = z_1^{-3} \int_0^{z_1} z^{2n+4} (z_1^2 - z^2)^{1/2} dz = z_1^{2n+3} g_2(n), \quad (A4)$$

$$g_4(n) = (1-z_2^2)^{-3/2} \int_{z_2}^1 z^{2n+1} (1-z^2)^{3/2} (z^2 - z_2^2)^{1/2} dz = (1-z_2^2)^{n+3/2} \sum_{k=0}^n (-1)^k \binom{n}{k} g_3(k). \quad (A5)$$