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**Brillouin-Zone Integration Schemes:
An Efficiency Study for the Phonon
Frequency Moments of the Harmonic,
Solid, One-Component Plasma**

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BRILLOUIN-ZONE INTEGRATION SCHEMES:
AN EFFICIENCY STUDY FOR THE PHONON FREQUENCY
MOMENTS OF THE HARMONIC, SOLID, ONE-COMPONENT PLASMA

by

R. C. Albers and J. E. Gubernatis

ABSTRACT

The efficiency of four different Brillouin-zone integration schemes including the uniform mesh, special point method, special directions method, and Holas method are compared for calculating moments of the harmonic phonon frequencies of the solid one-component plasma. Very accurate values for the moments are also presented. The Holas method for which weights and integration points can easily be generated has roughly the same efficiency as the special directions method, which is much superior to the uniform mesh and special point methods for this problem.

Brillouin zone integrations are required for calculating many properties of solids. Usually, such integrations cannot be done analytically, and an efficient, accurate, numerical procedure is necessary. Often, efficiency is of paramount importance since some calculations would otherwise be prohibitively expensive.

In the last twenty years, several new techniques have been devised, each with its proponents and critics. In practice, as explained below, the most appropriate technique for any given Brillouin zone integration can crucially depend on the integrand. While general theoretical guidelines can be established, the most efficient technique must usually be determined by a direct comparison of the results of the different integration schemes. It is therefore useful to develop test cases where the techniques have been applied and compared for different kinds of integrands. Over time, such tests will provide valuable information about the techniques and help future investigators more quickly decide which technique is best for their application.

In this report, we have used four Brillouin zone integration schemes (BZIS) for calculating moments of the phonon frequencies of the harmonic, solid, one-component plasma (OCP). These moments form a representative, but not a completely comprehensive set of different kinds of integrations required for the complete thermodynamic properties of phonon theories. For example, at high temperatures the displacement-displacement self-correlation function is proportional to the -2 moment and at zero temperature is proportional to the -1 moment. At zero temperature the zero-point energy contributions are proportional to the +1 moment.

Two unique features of the harmonic OCP make it an interesting test case. First, when the moments are scaled by the appropriate power of the plasma frequency ω_p ($= 4\pi ne^2/m$), they are independent of density and temperature.¹ Secondly, for the b.c.c. space lattice (the only one we consider) and other Bravais lattices, the longitudinal phonon mode goes to the plasma frequency instead of zero near the zone center ($q = 0$), see Fig. 1, and hence is more typical of an optical mode than an acoustical mode. Thus the OCP includes a phonon spectrum representative of more complex phonon theories which have more than one ion per unit cell.

We define the n th frequency moment as

$$\mu_n = \frac{1}{3N} \sum_{\vec{q}, j}^{\text{BZ}} \left[\frac{\omega(\vec{q}, j)}{\omega_p} \right]^n ,$$

where the phonon frequency of wavevector $\vec{q}$ and mode j is $\omega(\vec{q}, j)$ for the $3N$ normal modes in the Brillouin zone (BZ) for N ions.

We now sequentially consider the four different Brillouin zone integration schemes. In all cases we used the symmetry of the b.c.c. space lattice to reduce the full Brillouin zone integral to its 1/48th irreducible part.

I. UNIFORM MESH

This BZIS was the first numerical scheme to be implemented. While there are many different variations (which are mainly concerned with the appropriateness of including points along symmetry directions and at symmetry points), they all sample the integrand over a uniform mesh of $\vec{q}$ points in the irreducible part of the Brillouin zone. While this is the simplest and most straightforward approach to numerical integration, this technique does not take advantage of any characteristic feature of the integrand and hence is often slowly converging.

For our tests, we have used the algorithm of Wallace,² which is easy to program for a computer. It generates a mesh with values of

$$\vec{q} = (p_1, p_2, p_3) \left(\frac{1}{L_p} \right) (2\pi/a) , \quad (1)$$

where $0 \leq p_1, p_2, p_3 \leq L_p$ are integers such that $\vec{q}$ lies in the 1/48 th irreducible part of the zone. The integer L_p controls the fineness of the mesh.

For an arbitrary function $f(\vec{q})$ that has the symmetry of the lattice, we then have

$$\frac{1}{N} \sum_{\vec{q}}^{\text{BZ}} f(\vec{q}) = \sum_i w_i f(\vec{q}_i) , \quad (2)$$

where at each mesh point $\vec{q}_i$ there is a weighting factor W_i which is uniform except along symmetry directions and at symmetry points where it is reduced by an appropriate amount.² The weights are normalized by the condition

$$\sum_i W_i = 1 \quad . \quad (3)$$

In Table I, we show the convergence of the -2, -1, and 1 moments. The zero moment is not shown since Eq. (3) guarantees that it is unity to machine accuracy (approximately 14 significant figures). The second moment is also not shown since the Kohn sum rule,

$$\sum_{j=1}^3 \left| w(\vec{q}, j) / w_p \right|^2 = 1 \quad , \quad (4)$$

which is a special property of the harmonic, solid OCP, forces the -2 moment to be 1/3 to the same accuracy as the weight normalization.

Table I clearly shows the slow convergence of the uniform mesh for our application. The bottom row, labeled "estimate," is our best value for the various moments and was calculated by the methods to be described in Section IV.

II. SPECIAL POINT METHOD

The special point BZIS³⁻⁸ is a popular method since in many cases it leads to accurate Brillouin zone integrations with surprisingly few mesh points. It must, however, be handled with care. As we explain below, a straightforward application of this method to the harmonic, solid OCP led to unsatisfactory results.

The special point BZIS takes advantage of the translational symmetry in reciprocal lattice space of the integrands $f(\vec{q})$ which can therefore be expanded in the Fourier series

$$f(\vec{q}) = f_o + \sum_{m=1}^{\infty} f_m A_m(\vec{q}) \quad (5)$$

where

$$A_m(\vec{q}) = \sum_{|\vec{R}|=C_m} e^{i\vec{q} \cdot \vec{R}} \quad (6)$$

The $\vec{R}$ sum in (6) is over all lattice vectors related by the symmetry operations of the point group of the lattice. The index m in (5) and (6) is ordered so that the magnitudes $C_{m+1} > C_m$ for each shell m and $m + 1$.

The special point BZIS is a method for choosing a set of weights W_i and special points $\vec{q}_i$ such that Eq. (2) is satisfied exactly if the representation of Eq. (3) is exact when the sum over shells is truncated at some finite number. The error of the method ε for an arbitrary integrand can then be written as⁴

$$\varepsilon = \sum_{m>n} \varepsilon_m N_m f_m \quad (7)$$

where

$$\varepsilon_m = \pm 1 \text{ and}$$

$$N_m = \frac{1}{N} \sum_{\vec{q}}^{\text{BZ}} [A_m(\vec{q})]^2 \quad (8)$$

As more shells are exactly integrated, of course, the number of special points increases rapidly.

There are different ways to choose the special points and consequently there is some controversy over which choice guarantees the smallest number of points to sum a given number of shells. We have arbitrarily chosen the approach of Chadi and Cohen⁴; however, the qualitative problems of the method for the OCP should be similar for the others as well.

The difficulty of applying the special point BZIS results from the small $\vec{q}$ behavior in the integrands for the -2 and -1 moments. For the transverse modes $\omega(\vec{q}, j)$ is linear in q for small q and hence the integrand diverges as q^{-2} and q^{-1} . The moments, of course, remain finite because of the phase space factor q^2 :

$$\frac{1}{N} \sum_{\vec{q}}^{\text{BZ}} = \frac{V_c}{(2\pi)^3} \int_{\text{BZ}} q^2 dq \int d\Omega_{\hat{q}}, \quad (9)$$

where V_c is the volume of the unit cell and $d\Omega_{\hat{q}}$ is the solid angle differential. Straus⁹ has shown that if

$$\begin{aligned} \lim_{q \rightarrow 0} f(\vec{q}) = & \frac{1}{2} Q^{(-2)}(\hat{q}) + \frac{1}{q} Q^{(-1)}(\hat{q}) \\ & + Q^{(0)}(\hat{q}) + q Q^{(1)}(\hat{q}) + \dots, \end{aligned} \quad (10)$$

then

$$\begin{aligned} \lim_{m \rightarrow \infty} f_m = & \frac{1}{|\vec{R}_m|} F^{(-2)} + \frac{1}{|\vec{R}_m|^2} F^{(-1)} \\ & + \frac{1}{|\vec{R}_m|^3} F^{(0)} + \frac{1}{|\vec{R}_m|^4} F^{(1)} + \dots \end{aligned} \quad (11)$$

and hence the error estimate Eq. (7) may not converge or may converge very slowly for integrands proportional to q^{-2} and q^{-1} at small q .

Our results for the harmonic, solid OCP are consistent with this analysis as shown in Table II. The -2 moment appears not to converge. The -1 moment converges extremely slowly. Surprisingly, the +1 moment also converges slowly, although somewhat faster than the -1 moment.

In view of the success the special point BZIS has had for other systems, this study shows that the efficiency of a given BZIS can be strongly dependent on the integrand.

III. SPECIAL DIRECTIONS METHOD

Whereas the special point BZIS exploits the translational invariance symmetry properties of the crystal to develop an efficient integration technique, the special direction BZIS¹⁰⁻¹³ exploits the rotational symmetries of the point groups of the crystal. In this method the integration is rewritten as

$$\frac{v_c}{(2\pi)^3} \int_{\text{BZ}} d^3q f(\vec{q}) = \int \frac{v_c}{(2\pi)^3} d\Omega_{\hat{q}} \tilde{f}(\hat{q}) \quad (12)$$

where

$$\tilde{f}(\hat{q}) \equiv \int_0^{q_m(\hat{q})} dq q^2 f(q\hat{q}) \quad , \quad (13)$$

and $q_m(\hat{q})$ is the value of q at the Brillouin zone boundary in the direction $\hat{q}$. The evaluation of $\tilde{f}(\hat{q})$ is unspecified. The essence of the method is an efficient way of doing the solid angle integral. To do this, Fehlnner, et al.¹¹⁻¹² expanded $\tilde{f}(\hat{q})$ in terms of fully symmetric cubic harmonics and then found special directions and appropriate weights that will efficiently integrate as many cubic harmonics as possible. Consequently, the special direction BZIS will be most accurate when only a few cubic harmonics are needed to accurately represent $\tilde{f}(\hat{q})$.

The advantage of this method for the solid, harmonic OCP is that the factor of q^2 in Eq. (13) removes the divergence problems of the inverse moments and hence $\tilde{f}(\hat{q})$ can be very accurately determined by a Gaussian integration with as few as four or five radial points. As shown in Table III, the scheme works reasonably well for the small number of points used. However, since the algorithm to calculate the weights and directions is too complicated to be conveniently incorporated into a simple computer subroutine, use of the method presently requires the input of tables, which is somewhat tedious for a large number of points. For this reason, and since the efficiency of the method is comparable to those in Section IV, we did not bother to test the method up to the maximum number of available directions ($N_{\hat{q}} = 66$).¹³ We also note that

the accuracy of the tables is 12 significant figures, which is slightly less than the accuracy of our CDC 7600 computer (accurate to about 14 significant figures) and of the intrinsic accuracy of the other methods we studied.

IV. HOLAS METHOD

The Holas BZIS¹⁴ is similar to the special direction method in that it divides the Brillouin zone integral into radial and solid angle integrals. The evaluation of the solid angle integral, however, does not start with an expansion of $\tilde{f}(\vec{q})$ in terms of a specific symmetry compatible set of special functions, but instead immediately converts the integral into an equivalent integration over a set of triangles.

More explicitly, we wish to evaluate an integral of the form

$$\frac{1}{V_{ir}} \int_{IR} d^3q f(\vec{q}) \quad , \quad (14)$$

where V_{ir} is the volume of the irreducible part of the Brillouin zone, which is a tetrahedron with a vertex at the zone center and a right-triangular base on the zone face for the b.c.c. space lattice. For this case, Holas showed that (14) can be written as

$$6 \int_0^1 d\eta \int_0^\eta d\xi \int_0^1 d\xi \xi^2 f(\vec{q}(\xi, \eta, \xi)) \quad , \quad (15)$$

where

$$\vec{q} = (1 - \frac{1}{2}\eta, \frac{1}{2}\eta, \frac{1}{2}\eta + \frac{1}{2}\xi) \xi \frac{2\pi}{a} \quad . \quad (16)$$

The integration over ξ corresponds to integrating along a direction (specified by η and ξ) from the vertex of the tetrahedron to a point on the triangular base. The η and ξ integrals correspond to integrating over the triangular base.

At this point one can adopt several different approaches. Holas used a Gauss formula for the ξ integration and the symmetric triangular integration formulas described in Sec. 3 of Hammer et al.¹⁵ for the $\eta - \xi$

integrations. The latter represent the integral as the sum of weighted integrands over a set of N_p points ($N_p = 1, 3, 4$, and 7) affine-symmetrically distributed over the triangle:

$$\int_0^1 d\eta \int_0^\eta d\xi \phi(\eta, \xi) = \sum_{i=1}^{N_p} v_i \phi(\eta_i, \xi_i) \quad (17)$$

For higher accuracy, the triangle can be subdivided into four equal subtriangles of the same form, which in turn can be further subdivided. (see the Appendix). With suitable scaling of the parameters, formula (17) can then be applied to each of the subtriangles. We will arbitrarily call this approach the "Holas method." The final integration formula is

$$6 \sum_i \sum_j g_i v_j \xi_i^2 f(\vec{q}(\xi_i, \eta_j, \xi_j)) \quad (18)$$

where the weights g_i and points ξ_i are those of a Gaussian integration formula for an interval 0 to 1:

$$\int_0^1 d\xi f(\xi) = \sum_i g_i f(\xi_i) \quad (19)$$

As an alternative, we have considered the triangular integration scheme developed in Sec. 2 of Hammer et al.¹⁵ This is most easily explained if we redefine the ξ variable and rewrite (15) as

$$6 \int_0^1 \eta d\eta \int_0^1 d\xi \int_0^1 d\xi \xi^2 f(\vec{q}(\xi, \eta, \eta\xi)) \quad (20)$$

It is then possible to use the Gaussian formula (19) for the ξ and ξ integrations. The η integration is done with a generalized Gaussian formula with a weight function η :

$$\int_0^1 \eta d\eta f(\eta) = \sum_i w_i f(\eta_i) \quad (21)$$

Hammer et al.¹⁵ provide some tables for the weights and points w_i and η_i .

Alternatively, at Los Alamos, one can use the computer subroutine GENGSQ¹⁶ to generate these weights and points. The final integration formula for this approach, which we will call the "generalized Gaussian Holas method," is

$$6 \sum_i \sum_j \sum_k g_i w_j g_k \xi_i^2 f(\vec{q}(\xi_i, \eta_j, \eta_j \xi_k)) \quad (22)$$

Since generalized Gaussian subroutines are not widely accessible, we have also considered doing the n integration with the Gaussian formula (19). The integration formula for this approach, which we will call the "Gaussian Holas method," is

$$6 \sum_i \sum_j \sum_k g_i g_j g_k \xi_i^2 \eta_i f(\vec{q}(\xi_i, \eta_j, \eta_j \xi_k)) \quad (23)$$

In addition, we have also examined a similar procedure which we will call the "variant Holas method," that is equivalent to integrating over a triangle in the plane $q_x = 1$ (in units of $2\pi/a$) instead of the right-triangular base of the Brillouin zone face which Holas used. This corresponds to a change of variables

$$\vec{q} = (1, \eta, \xi) \frac{\xi}{1 + \eta} \left(\frac{2\pi}{a} \right) \quad (24)$$

where (15) becomes

$$24 \int_0^1 d\eta \frac{\eta}{(1 + \eta)^3} \int_0^1 d\xi \int_\infty^1 d\xi \xi^2 f(\vec{q}(\xi, \eta, \eta \xi)) \quad (25)$$

For the ξ and ζ integrals, we used the Gaussian formula (19). For the η integral, we used the computer subroutine GENGSQ with the weighting function $\eta(1 + \eta)^{-3}$ to generate the points and weights

$$\int_0^1 d\eta \frac{\eta}{(1 + \eta)^3} f(\eta) = \sum_i u_i f(\eta_i) \quad (26)$$

The final integration is

$$24 \sum_i \sum_j \sum_k g_i u_j g_k \xi_i^2 f(\vec{q}(\xi_i, \eta_j, \eta_j, \xi_k)) \quad (27)$$

As with all the different Holas variations, the accuracy can be increased by subdividing the $\eta - \xi$ triangle.

Up to this point, we have not discussed the role of the ξ integration in the Holas approach. In principle, we are not limited to the single Gaussian formula (19). With the availability of GENGSQ, we have the flexibility of doing this integral by using

$$\int_0^1 d\xi W(\xi) \frac{f(\xi)}{W(\xi)} = \sum_i a_i \left[\frac{f(\xi_i)}{W(\xi_i)} \right] \quad (28)$$

where the weighting function $W(\xi)$ can be chosen to optimize the efficiency of the integral. For the moments of the OCP, we tried $W(\xi) = \xi^{\frac{1}{2}}, 1, \xi^1, \xi^2$, and ξ^3 . The weight function $W(\xi) = 1$, which is identical with the Gaussian formula (19) seemed to work best.

Holas¹⁴ suggested the possibility of subdividing the integral $[0,1]$ into subintervals of decreasing length near the origin:

$$[0,1] = [0,p^{N-1}] + [p^{N-1},p^{N-2}] + \dots + [p^1,p^0]$$

where the parameter p is the ratio of the scaling intervals ($p < 1$). This scheme is useful for integrands that have significant structure near $\xi = 0$. We also applied this method to the moments of the OCP and concluded that it did not improve the accuracy of the ξ integral. Thus, all the results we report for the different Holas methods used the simple Gaussian formula for the ξ integral.

The results for the OCP moments are given in Tables IV to VII. All variations of the Holas method have comparable efficiency, and all moments converge in a satisfactory manner. Clearly, the Holas BZIS is a flexible and valuable approach for numerical Brillouin zone integrations. Our best estimate for the moments, which we used in Tables I-III, are derived from the Holas results.

APPENDIX SUBDIVISION INTO SUBTRIANGLES

We present here an algorithm for subdividing the $\eta - \xi$ triangle into four subtriangles and show how this algorithm may be cycled in a particularly simple way to repeatedly subdivide each subtriangle into four additional subtriangles.

To start, we assume that we have an integration formula of N_p weights and points for the right triangle defined by the points $(0,0)$, $(1,0)$, and $(1, 1)$, i.e.,

$$\int_0^1 dx \int_0^x dy f(x, y) = \sum_{i=1}^{N_p} v_i f(x_i, y_i) \quad . \quad (A1)$$

As it stands, we could apply this formula directly to the integral we wish to evaluate

$$\int_0^1 d\eta \int_0^\eta d\xi f(\eta, \xi) \quad . \quad (A2)$$

Instead we wish to scale (A1) in such a way that it can be used for integration over four subtriangles, which can then be summed to evaluate (A2).

To do this we define the four equal right triangles of Fig. 2. If $(x^{(\mu)}, y^{(\mu)})$ is a point in the μ th triangle, then we want the transformation of coordinates such that

$$\int_0^1 d\eta \int_0^\eta d\xi = \frac{1}{4} \sum_{\mu=1}^4 \int_0^1 dx^{(\mu)} \int_0^{x^{(\mu)}} dy^{(\mu)} \quad . \quad (A3)$$

From Fig. 2, this is

$$\begin{aligned}
 \eta &= \frac{1}{2}x^{(1)} & \xi &= \frac{1}{2}y^{(1)} \\
 \eta &= 1 - \frac{1}{2}x^{(2)} & \xi &= \frac{1}{2}y^{(2)} \\
 \eta &= 1 - \frac{1}{2}y^{(3)} & \xi &= \frac{1}{2}y^{(3)} \\
 \eta &= \frac{1}{2}(1 + x^{(4)}) & \xi &= \frac{1}{2}(1 + y^{(4)})
 \end{aligned} \tag{A4}$$

Thus the final integration formula for the complete triangle is

$$\int_0^1 d\eta \int_0^\eta d\xi f(\eta, \xi) = \sum_{\mu=1}^4 \sum_{i=1}^N (\frac{1}{2}v_i) f(\eta(x_i^{(\mu)}, y_i^{(\mu)}), \xi(x_i^{(\mu)}, y_i^{(\mu)})) \tag{A5}$$

where $\eta(x_i^{(\mu)}, y_i^{(\mu)})$ and $\xi(x_i^{(\mu)}, y_i^{(\mu)})$ are given by the trans-

formation equations (A4). Clearly (A5) can be rewritten as

$$\int_0^1 d\eta \int_0^\eta d\xi f(\eta, \xi) = \sum_{j=1}^N w_j f(\eta_j, \xi_j) \tag{A6}$$

To continue this process, one could explicitly divide each of the four subtriangles of Fig. 2 into four additional subtriangles and replace (A3) by

$$\int_0^1 d\eta \int_0^\eta d\xi = 1/16 \sum_{\mu=1}^{16} \int_0^1 dx^{(\mu)} \int_0^{x^{(\mu)}} dy^{(\mu)} \tag{A7}$$

and replace (A4) with 16 sets of transformation formulae. This would obviously be a tedious procedure, especially at the next stage of 64 triangles.

However, there is a much simpler alternative: After each cycle, replace the weights and points of (A1) by those of (A6), and then reuse the transformation formulae of (A3) to (A5) to generate new weights and points. Then the subdivision is done automatically. This algorithm is shown schematically in Fig. 3, where we indicate the original integration points of (A1) by three closely spaced points and sketch the integration points of two successive cycles.

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TABLE I
UNIFORM MESH

N is the total number of points used in the integration formula and L_p is defined in Eq. (1).

N	L_p	μ_{-2}	μ_{-1}	μ_1
90	10	12.244517	2.7888754	0.51146889
139	12	12.355717	2.7915504	0.51143542
284	16	12.503217	2.7944498	0.51140809
505	20	12.594877	2.7958729	0.51139814
818	24	12.656902	2.7966685	0.51139369
1014	26	12.680912	2.7969399	0.51139237
1495	30	12.719480	2.7973326	0.51139067
ESTIMATE		12.973000	2.7985600	0.51138740

TABLE II
SPECIAL POINT METHOD

N is the total number of points used in the integration formula.

N	μ_{-2}	μ_{-1}	μ_1
1	7.6143524	2.4967868	0.51570695
2	8.0797328	2.5599056	0.51402631
8	17.869787	2.3503474	0.49204634
40	22.062505	3.2648903	0.50486956
240	22.740070	3.1172776	0.50821811
1632	20.942651	2.9838704	0.50974809
ESTIMATE	12.973000	2.7985600	0.51138740

TABLE III
SPECIAL DIRECTIONS

N is the total number of integration points, N_q the number of radial points, and $N_{\hat{q}}$ the number of directions.

N	N_q	$N_{\hat{q}}$	μ_{-2}	μ_{-1}	μ_1
16	4	4	12.802889	2.7366096	0.49363424
64	16	4	12.802927	2.7366131	0.49363516
24	4	6	12.942730	2.8196058	0.51827878
40	4	10	12.988649	2.8165997	0.51689621
60	4	15	12.999701	2.8130973	0.51561221
84	4	21	12.995004	2.8092517	0.51448915
336	16	21	12.995102	2.8092625	0.51448877
ESTIMATE			12.973000	2.7985600	0.51138740

TABLE IV
HOLAS METHOD

N is the total number of integration points, N_q is the number of radial points used in the ξ integration, $N_{\hat{q}}$ is the total number of directions used in the $\eta - \zeta$ integral, N_p is the number of affine-symmetric points used for each subtriangle, and N_T is the number of subtriangles used.

N	N_q	$N_{\hat{q}}$	N_p	N_T	μ_{-2}	μ_{-1}	μ_1
4	4	1	1	1	12.600797	2.8731919	0.50373123
12	4	3	3	1	13.180278	2.8097293	0.51139250
16	4	4	1	4	12.230489	2.7571867	0.51168836
16	4	4	4	1	12.992982	2.7848841	0.51254379
28	4	7	7	1	13.041751	2.8025417	0.51130414
48	4	12	3	4	13.059893	2.8043411	0.51127068
64	4	16	1	16	12.920850	2.7975058	0.51126670
64	4	16	4	4	13.041151	2.8047668	0.51120226
112	4	28	7	4	12.996118	2.7994626	0.51138842
192	4	48	3	16	12.989633	2.7992421	0.51138367
256	4	64	1	64	12.977181	2.7990433	0.51135283
256	4	64	4	16	12.991264	2.7993322	0.51138262
448	4	112	7	16	12.972682	2.7985344	0.51138772
768	4	192	3	64	12.973097	2.7985529	0.51138755
1152	6	192	3	64	12.973185	2.7985617	0.51138741
1536	8	192	3	64	12.973186	2.7985618	0.51138742
1024	4	256	4	64	12.973157	2.7985554	0.51138752
1536	6	256	4	64	12.973245	2.7985641	0.51138738

TABLE V
GENERALIZED GAUSSIAN HOLAS METHOD

N is the total number of integration points, N_q is the number of radial points used for the ξ integration, $N_{\hat{q}}$ is the number of radial points used for the ξ integration, $N_{\hat{q}}$ is the total number of directions used in the integral over the $\eta - \xi$ triangle.

N	N_q	$N_{\hat{q}}$	μ_{-2}	μ_{-1}	μ_1
64	4	16	13.013531	2.8014714	0.51133877
125	5	25	12.951436	2.7968706	0.51141301
144	4	36	12.976862	2.7990259	0.51137934
256	4	64	12.973452	2.7985904	0.51138703
400	4	100	12.972701	2.7985355	0.51138765
784	4	196	12.972797	2.7985420	0.51138760
1568	8	196	12.972886	2.7985509	0.51138747

TABLE VI
GAUSSIAN HOLAS METHOD

N is the total number of integration points, N_q is the number of radial points used for the ξ integral, $N_{\hat{q}}$ is the total number of directions used in the integral over the $\eta - \xi$ triangle.

N	N_q	$N_{\hat{q}}$	μ_{-2}	μ_{-1}	μ_1
64	4	16	13.073902	2.8062736	0.51121572
125	5	25	12.957558	2.7969324	0.51142330
144	4	36	12.969643	2.7985293	0.51138422
256	4	64	12.971549	2.7984462	0.51138864
400	4	100	12.972492	2.7985191	0.51138782
784	4	196	12.972812	2.7985429	0.51138759
1568	8	196	12.972901	2.7985518	0.51138746

TABLE VII
VARIANT HOLAS METHOD

N is the total number of integration points, N_q is the number of radial points used for the ξ integral, $N_{\hat{q}}$ is the total number of directions used in the integral over the $\eta - \xi$ triangles, N_T is the number of subtriangles used in the directional integration.

N	N_q	$N_{\hat{q}}$	N_T	μ_{-2}	μ_{-1}	μ_1
64	4	16	1	12.927578	2.7947780	0.51144034
125	5	25	1	12.984959	2.7995636	0.51137679
144	4	36	1	12.969010	2.7982584	0.51138984
256	4	64	1	12.972593	2.7985351	0.51138745
256	4	64	4	12.971414	2.7984646	0.51138807
400	4	100	1	12.972771	2.7985470	0.51138752
600	6	100	4	12.972876	2.7985541	0.51138738
784	4	196	1	12.972813	2.7985429	0.51138759
784	4	196	4	12.972804	2.7985423	0.51138760
1568	8	196	1	12.972901	2.7985518	0.51138746
1536	6	256	4	12.972892	2.7985512	0.51138745

Fig. 1. Harmonic phonon frequencies of the solid one-component plasma along a direction whose end point is $(1, 1/10, 1/10) 2\pi/a$. Frequencies are in units of the plasma frequency ω_p and wave-vectors in units of the magnitude of the end point $q_{\max}$.

Fig. 2. Subdivision of the η - ζ triangle into four subtriangles.

Fig. 3. A schematic drawing of the integration points of (A1) and of two successive cycles of the subdivision algorithm.