

## High-precision sampling for Brillouin-zone integration in metals

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We present a sampling method for Brillouin-zone integration in metals which converges exponentially with the number of sampling points, without the loss of precision of normal broadening techniques. The scheme is based on smooth approximants to the  $\delta$  and step functions which are constructed to give the exact result when integrating polynomials of a prescribed degree. In applications to the simple-cubic tight-binding band as well as to band structures of simple and transition metals, we demonstrate significant improvement over existing methods. The method promises general applicability in the fields of total-energy calculations and many-body physics.

### I. INTRODUCTION

In solid-state one-electron and many-body calculations, integrals of periodic functions over the Brillouin zone (BZ) are routinely made in the evaluation of densities of states, single-particle sums, charge densities, matrix elements, response functions, and so on. Precision in energy on the order of 1 mRy is common; in more demanding cases, such as the calculation of phonon frequencies, one requires 1 or 2 orders of magnitude better convergence. In the case of insulators and semiconductors, the function to be integrated has the property that it is infinitely many times differentiable, due to the separation of occupied and empty bands by a gap. Under these circumstances, it is well known<sup>1</sup> that integrals converge exponentially in  $h$ , where  $h$  is the spacing between divisions made along the primitive vectors of the reciprocal lattice in constructing a uniform mesh over the BZ. (By exponential convergence, we mean convergence that is more rapid than any power in  $h$ .) Investigations into the properties of metals, on the other hand, are hampered by the fact that one must integrate a function over the BZ that is discontinuous due to the partial filling of the energy bands, and hence not even once differentiable. This leads to very slow convergence when sampling over a uniform mesh in the BZ, or at best an  $h^2$  convergence<sup>2</sup> when using the linear tetrahedron method.<sup>3</sup> Since in many applications the time-limiting procedure is the solution to an eigenvalue problem at each sampling  $\mathbf{k}$  point, it is important that the required precision be obtained without a prohibitively fine  $\mathbf{k}$  mesh.

We will implicitly deal with two types of convergence in what follows, which may be best illustrated by reference to a very commonly used procedure for BZ integration in metals: one may immediately obtain improved  $\mathbf{k}$  convergence by a broadening or "smearing" of contributions from all  $\mathbf{k}$  points into Gaussian, Lorentzian, or similar smooth functions with characteristic linewidth  $W$  (thorough discussions can be found in Refs. 4 and 5). This method ensures exponential convergence of integrals, albeit to the wrong answer. The only justification for this *ad hoc* procedure is that in the limit as  $W \rightarrow 0$  one would recover the "absolutely" converged result—at the

expense of using a prohibitively fine  $\mathbf{k}$  mesh. Thus for each choice of  $W$  the broadening method will converge to a particular result; in the unattainable limit as  $W \rightarrow 0$  so would each of these results converge absolutely to the precise answer.

It is our intention to show here that a more sophisticated choice of the broadening function can provide the necessary freedom with which to control both the  $\mathbf{k}$  convergence and the absolute convergence independently. In practice, this means that a broadening can be chosen for which  $\mathbf{k}$  convergence is reached for a relatively coarse mesh *and* that the corresponding limit is close to the true value. The method we propose revolves around a hierarchy of smooth approximations to the step and  $\delta$  functions, which we derive and motivate in the following two sections. These are then applied to BZ integrals for the simple-cubic tight-binding band in Sec. IV and to actual band structures of metals in Sec. V. The most important points are summarized in Sec. VI.

### II. SMOOTH APPROXIMATIONS TO THE STEP AND $\delta$ FUNCTIONS

We wish to evaluate

$$I = \int_{\text{BZ}} S(E(\mathbf{k}) - E_F) f(\mathbf{k}) d\mathbf{k} = \int_{-\infty}^{\infty} S(\epsilon - E_F) F(\epsilon) d\epsilon,$$

where

$$F(\epsilon) = \int_{\text{BZ}} f(\mathbf{k}) \delta(\epsilon - E(\mathbf{k})) d\mathbf{k}.$$

$E(\mathbf{k})$  represents an energy band as a function of wave vector and  $E_F$  is the Fermi energy. The function to be integrated,  $f$ , is multiplied by the Fermi cutoff or step function:  $S(x) = 1 - \Theta(x) = 1$  for  $x \leq 0$ , and 0 otherwise.  $F(\epsilon)$  might be, for example, the density of states  $g(\epsilon)$ , if  $I$  is to be the total charge within the Fermi surface; or  $F(\epsilon) = g(\epsilon)\epsilon$  if  $I$  is to be the band energy. It is easy to see that conventional smearing, which essentially replaces  $S(x)$  by a Fermi-Dirac-like distribution, leads to an error in the integration which is shown schematically in Fig. 1. Note that in general this will occur unless  $F(\epsilon)$  is a constant near  $E_F$ .

The more sophisticated approach we adopt amounts to

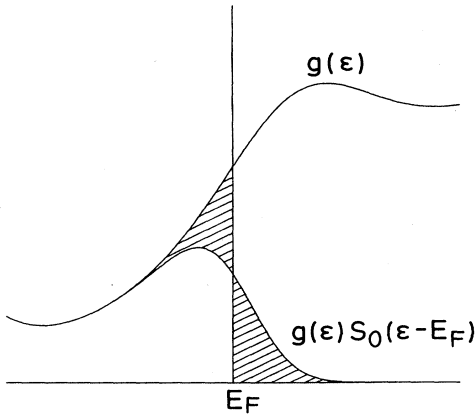


FIG. 1. A schematic density of states  $g(\epsilon)$  and the same function multiplied by a Fermi-Dirac-like smoothing. An error arises when the charge below  $E_F$  is calculated as  $\int g(\epsilon)S_0(\epsilon-E_F)d\epsilon$  since the two hatched areas are not equal, unless the density is constant near  $E_F$ .

a search for successive approximants,  $S_N$ , to the step function which are smooth and for which the error is zero if  $F(\epsilon)$  is a polynomial of some order within the energy range determined by the choice of broadening. If we use a characteristic broadening  $W$ , we can work with a dimensionless energy variable,  $x = (\epsilon - E_F)/W$ , and look for a function  $S_N(x)$  to approximate  $S(x)$ . Our approach is to write down a suitable representation of the  $\delta$  function  $\delta(x)$ , which we will integrate to obtain successive approximants to  $S(x)$ . One may expand  $\delta(x)$  in a complete set of functions, and since it is even we may write,

$$\delta(x) = \sum_{n=0}^{\infty} A_n H_{2n}(x) e^{-x^2},$$

where  $H_n$  is the Hermite polynomial<sup>1,6</sup> of degree  $n$ . Using the orthogonality of the Hermite polynomials with respect to Gaussian weights:

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = n! 2^n \sqrt{\pi} \delta_{nm},$$

we obtain for the coefficients  $A_n$ ,

$$A_n = \frac{H_{2n}(0)}{(2n)! 4^n \sqrt{\pi}} = \frac{(-1)^n}{n! 4^n \sqrt{\pi}}.$$

Now consider the finite sum

$$D_N(x) = \sum_{n=0}^N A_n H_{2n}(x) e^{-x^2}$$

which we introduce here as an approximation to the  $\delta$  function. By construction,

$$\int_{-\infty}^{\infty} D_N(x) P(x) dx = \int_{-\infty}^{\infty} \delta(x) P(x) dx = P(0)$$

if  $P(x)$  is a polynomial of degree  $2N+1$  or less; since then  $P(x)$  may be expanded in the Hermite polynomials up to degree  $2N+1$ . To obtain an approximation to the step function  $S(x)$ , we integrate  $D_N$ :

$$S_N(x) = 1 - \int_{-\infty}^x D_N(t) dt,$$

and making use of the identity  $(d/dx)[H_n(x)e^{-x^2}] = -H_{n+1}(x)e^{-x^2}$  and the definition of the error function,<sup>1</sup> we obtain the central result of the present paper:

$$S_0(x) = \frac{1}{2}(1 - \operatorname{erf}x)$$

$$S_N(x) = S_0(x) + \sum_{n=1}^N A_n H_{2n-1}(x) e^{-x^2}$$

in which the zero-order approximation  $S_0$  corresponds to simple Fermi-Dirac-like smearing, and higher-order terms serve to correct the errors inherent in such a procedure.

$S_N$  has a similar property as  $D_N$  of integrating polynomials exactly, since by partial integration of

$$0 = \int_{-\infty}^{\infty} [D_N(x) - \delta(x)] P(x) dx,$$

one has

$$0 = \int_{-\infty}^{\infty} [S_N(x) - S(x)] \frac{dP}{dx} dx.$$

Therefore,  $S_N(x)$  can be substituted for  $S(x)$  in the integral  $\int S(x)F(x)dx$  without incurring significant error if  $F(x)$  can be represented as a polynomial of degree  $2N$  or less in the range where  $S_N(x) - S(x)$  (or, equivalently,  $e^{-x^2}$ ) is appreciably nonzero; whereas  $S_0$  will serve only in cases where  $F(x)$  is constant in this interval. This is our desired property.

In Fig. 2 we show successive approximations  $S_N(x)$  and  $D_N(x)$  to the step function and  $\delta$  function, respectively. Note that both oscillate close to  $x=0$  as might be expected from the Gibbs phenomenon of Fourier

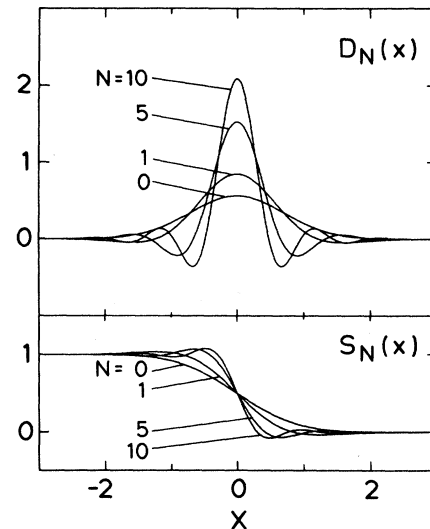


FIG. 2. Successive approximants to the  $\delta$  function,  $D_N$ , and to the step function  $S_N$ . The order of the approximant  $N$  is indicated on each curve. Note that the zero-order approximants are a Gaussian and complementary error function, respectively.

analysis. The figure shows that for practical purposes,  $D_N(x) \approx 0$  and  $S_N(x) \approx S(x)$  if  $|x|$  is greater than 2–3.

We remark that the method is trivially easy to include in a standard BZ sampling or special points<sup>7</sup> program. The approximants  $S_N(x)$  may be obtained using the recurrence for the Hermite polynomials:

$$H_0(x) = 1, \quad H_1(x) = 2x,$$

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

Substituting  $S_N(x)$  for  $S(x)$  in our original integral  $I$ , and sampling over a uniform mesh which is reduced by symmetry to a set of points  $\{\mathbf{k}_i\}$  with weight factors  $a_i$  in the irreducible wedge of the BZ, we obtain the quadrature

$$I_N \approx \sum_i a_i f(\mathbf{k}_i) S_N(x_i), \quad x_i = \frac{E(\mathbf{k}_i) - E_F}{W}.$$

The sum converges exponentially in  $\mathbf{k}$  space because of the smoothness of  $S_N$ . This procedure is as simple as conventional broadening methods for metals. In fact such a method is equivalent to our zero-order approximation with  $W$  equal to the width of broadening used. If  $D_N/W$  is substituted for  $S_N$  in the above equation, one obtains a completely analogous method for evaluating integrals over the Fermi surface. We remark in passing that  $S_N$  and  $D_N$  could be used in other contexts, for integrating or interpolating a function of a single variable tabulated on a regular mesh.

To conclude this section, we note for completeness that the special integrative property of  $D_N$  and  $S_N$ , namely that they integrate polynomials up to a certain degree exactly, is not sufficient to define these functions uniquely. A similar formalism would result for another choice of weight function instead of the Gaussian. However, it is clear that for the application of integrating bands of arbitrary width with a step or  $\delta$  function at  $E_F$ , the weight function must be smooth over the whole real axis and strongly localized near  $x=0$ . It is convenient that the simplest choice, a Gaussian, is also the weight function for a convenient and well-known orthogonal-polynomial sequence.

### III. THE BENEFIT FROM USING HIGHER-ORDER APPROXIMANTS

For the  $\mathbf{k}$ -space integration procedure which we are presenting here, it is a complication that two parameters  $W$  and  $N$  must be chosen suitably. We would like to acquire a feeling for their significance. By construction, use of  $S_N$  (or  $D_N$ ) leads to a negligible error if  $F(\epsilon)$  is representable as a polynomial of degree  $2N$  (or  $2N+1$ ) or less in an interval of  $\sim 5W$  around the Fermi energy (see Fig. 2). The  $\mathbf{k}$ -space converged result can therefore be made to approach the true value either by increasing  $N$  or by reducing  $W$ . Obviously, our approach would be superfluous if it were always possible to reproduce the result for some set  $W$  and  $N$ , with equally fast  $\mathbf{k}$  convergence, by simply using the zero-order function at a smaller broadening. In this section, we show that the use of orders  $N > 0$  brings definite advantages which cannot be

simulated with zero-order functions.

Consider the simplest case for which  $S_1$  could give better results than  $S_0$ : as above, we want to integrate  $f(\mathbf{k})$  over the occupied part of the band, and we suppose that  $F(\epsilon)$  is linear in  $\epsilon$  near the Fermi energy  $E_F$ . The error in the integral obtained at  $\mathbf{k}$  convergence can be calculated by a standard integration, giving

$$\begin{aligned} \Delta I_N &= \int_{-\infty}^{\infty} \left[ S_N \left[ \frac{\epsilon - E_F}{W} \right] - S(\epsilon - E_F) \right] F(\epsilon) d\epsilon \\ &= \begin{cases} \frac{1}{4} F'(E_F) W^2 & \text{for } N=0 \\ 0 & \text{for } N>0. \end{cases} \end{aligned}$$

In this, and in what follows, primes denote differentiation with respect to  $\epsilon$ . One sees that the zero-order result converges to the correct value as  $W \rightarrow 0$ , but only as slowly as  $W^2$ . For the case under consideration, all higher-order approximants already give the exact result. The tests in Secs. IV and V will show that  $\mathbf{k}$  convergence is only marginally slower for  $S_1$  compared to  $S_0$ . Thus, there is an immediate gain in using  $S_1$  instead of  $S_0$  whenever  $F(\epsilon)$  has a nonzero linear term near  $E_F$ .

Next we determine the analogous relation for the case of an integral over the Fermi surface, i.e.,

$$J_N = \int_{-\infty}^{\infty} F(\epsilon) \frac{1}{W} D_N \left[ \frac{\epsilon - E_F}{W} \right] d\epsilon$$

which converges to  $F(E_F)$  as  $W \rightarrow 0$  or as  $N \rightarrow \infty$ . Since  $D_0$  integrates polynomials of linear order exactly,  $F(\epsilon)$  must have a nonvanishing quadratic term near  $E_F$  if  $D_1$  is to give a better result. If  $F(\epsilon)$  is quadratic in  $\epsilon$ , the error in  $J_N$  at  $\mathbf{k}$  convergence is

$$\Delta J_N = \begin{cases} \frac{1}{4} F''(E_F) W^2 & \text{for } N=0 \\ 0 & \text{for } N>0. \end{cases}$$

Again, we have found that  $\mathbf{k}$  convergence of integrals made using  $D_1$  is only slightly slower than those using  $D_0$ . The criterion for making Fermi-surface integrals is, therefore, use of  $D_1$  in place of  $D_0$  gives an immediate improvement if  $F(\epsilon)$  has a substantial quadratic term at  $E_F$ . As a practical example, note that an approximation to the density of states (DOS) for a given set of bands  $E_n(\mathbf{k})$  can be accumulated by adding  $D_N(x_{n,i})/W$ ,  $x_{n,i} = [\epsilon - E_n(\mathbf{k}_i)]/W$ , with the proper weight into the DOS for each band  $n$  and each mesh point  $\mathbf{k}_i$ . This is equivalent to the case under discussion if one considers  $E_F$  as a variable. From the expression for the error  $\Delta J_N$ , it follows that the use of  $D_0$ , i.e., making the DOS by conventional Gaussian smearing, has the effect of reducing peaks and filling in valleys, and that this undesirable phenomenon vanishes only as  $W^2$ . On the other hand, the DOS made using  $D_1$  will have the proper heights and depths if  $W$  is no larger than about one-tenth of the distance between successive peaks. For a larger broadening, the same improvement can be obtained through the use of functions of higher order than  $N=1$ . Tests for energy bands of transition metals have confirmed this.

The connection between the two cases (integrals over

the occupied states and over the Fermi surface) can be made in the following way. It is easy to show that

$$\int_{-\infty}^{\infty} F(\epsilon) S_N \left[ \frac{\epsilon - E_F}{W} \right] d\epsilon = \int_{-\infty}^{E_F} \bar{F}(\epsilon) d\epsilon ,$$

where  $\bar{F}(\epsilon)$  is the result of smoothing  $F(\epsilon)$  by convoluting it with  $D_N/W$ :

$$\bar{F}(\epsilon) = \int_{-\infty}^{\infty} F(t) \frac{1}{W} D_N \left[ \frac{\epsilon - t}{W} \right] dt .$$

It follows that  $\bar{F}(\epsilon)$  made using  $D_0$  is equal to  $F(\epsilon)$  at those energies for which  $F(\epsilon)$  is linear in  $\epsilon$  on the scale given by  $W$ . On the other hand, the integral up to  $E_F$  made using  $S_0$  is already in error if  $F(\epsilon)$  has a linear term, i.e., unless  $F(\epsilon)$  is approximately constant near  $E_F$ . The reason for this seeming discrepancy is that the integral has summed the errors in  $\bar{F}(\epsilon)$  for all energies up to  $E_F$ . The preceding equations show an interesting fact, namely that this accumulated error made by smoothing  $F(\epsilon)$  into  $\bar{F}(\epsilon)$  depends only on the behavior of  $F(\epsilon)$  near  $E_F$ . More precisely, the error estimate above gives this sum (to leading order) as proportional to the slope of  $F(\epsilon)$  at  $E_F$ .

#### IV. THE SIMPLE-CUBIC TIGHT-BINDING BAND

The tight-binding band (TB) on a simple-cubic lattice,

$$E(\mathbf{k}) = -\frac{1}{3}(\cos\pi k_x + \cos\pi k_y + \cos\pi k_z) ,$$

provides us with an ideal DOS  $g_{\text{TB}}(\epsilon)$  with which to both illustrate and test the principles of the present integration method. Near the minimum of the band at  $\epsilon = -1$ ,  $g_{\text{TB}}(\epsilon)$  shows free-electron-like behavior; near the center at  $\epsilon = 0$ , it is practically constant, and there are Van Hove singularities at  $\epsilon = \pm\frac{1}{3}$  and  $\pm 1$ . These features are seen in Fig. 3, where we also show the effect of convoluting  $g_{\text{TB}}(\epsilon)$  with  $\delta$ -function approximants of various orders. As expected, the convoluted DOS approaches the true DOS as  $N$  increases. Near the singularity at  $\epsilon = -\frac{1}{3}$ , the convoluted DOS has structure similar to the corresponding step-function approximant. The benefit gained through use of the higher-order functions is evident when compared with the zero-order approximation both where the DOS deviates from linearity and near the singularity. In the regions where the DOS is almost linear, all orders work equally well. The smoothing near the singularity is reduced if a smaller broadening is used; then  $S_N(x)$  varies more strongly in  $\mathbf{k}$  space and a finer  $\mathbf{k}$  mesh is needed. Thus the choice of broadening is determined by the distance of  $E_F$  from the Van Hove singularities and by the amount of variation of the DOS near  $E_F$ . The order  $N$  is determined by the required precision: small  $N$  requires fewer  $\mathbf{k}$  points at the expense of convergence to a less-precise result, higher orders guarantee convergence to the correct result but require more  $\mathbf{k}$  points.

For three choices of  $E_F$ , Fig. 4 illustrates the  $\mathbf{k}$  convergence of the charge within the Fermi surface using the present method and the linear tetrahedron method.

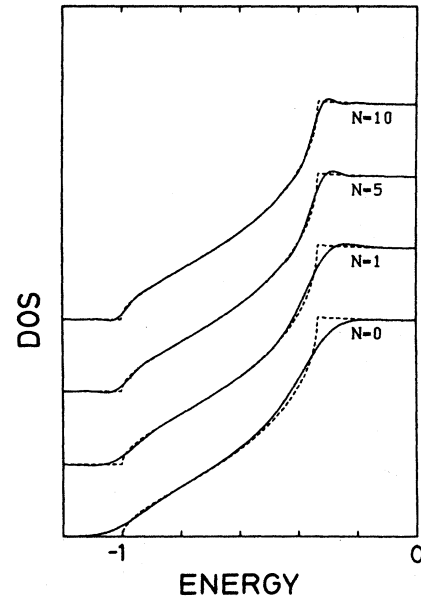


FIG. 3. Density of states of the simple cubic tight-binding band (Ref. 8) (dashed line) and successive approximations obtained from its convolution with approximants  $D_N$  to the  $\delta$  function. Only the negative energy range is shown. The energy broadening  $W$  is 0.10.

Characteristic for the curves made by sampling using the  $S_N$  is that they become flat very rapidly after a threshold for the fineness of the mesh is reached. For larger  $N$  the threshold is reached later. A more exact analysis shows that each curve converges to its limit as  $\exp(-C/h^2)$  whereas the linear method converges as  $h^2$ . In view of

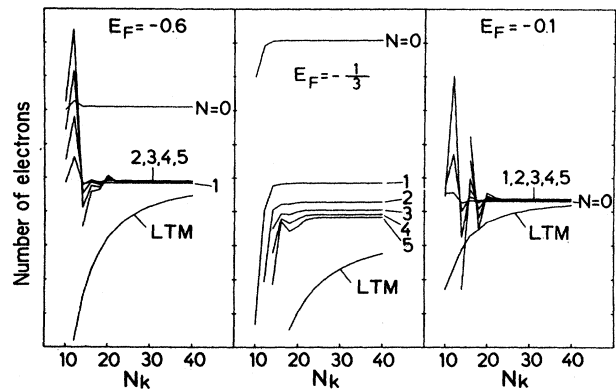


FIG. 4. The  $\mathbf{k}$  convergence of the charge within the Fermi surface for the simple-cubic tight-binding band for three choices of  $E_F$  as indicated.  $N_k$  is the number of divisions along each reciprocal lattice vector.  $N_k = 10$  and 40 correspond to 56 and 171 irreducible  $\mathbf{k}$  points, respectively; LTM denotes linear tetrahedron method; other curves result from successive approximations  $S_N$ . Each division on the ordinate represents 0.001 electrons (the band is normalized to one electron). The energy broadening is 0.10.

the considerations of Secs. II and III, the value to which the  $N$ th curve converges should depend on the shape of the DOS near the Fermi energy. In the first panel,  $E_F$  lies in the free-electron part of the band where the DOS has a large variation. Consequently, there is a marked improvement using  $S_N$  with  $N$  larger than zero. The DOS is very flat near  $E_F$  for the third panel, so that here  $S_0$  is already adequate. Finally, the second panel shows the result when  $E_F$  is chosen exactly on a Van Hove singularity. While convergence with increasing  $N$  is now slower, the advantage of using a higher-order  $S_N$  is obvious and the present approach still compares favorably with the linear method.

### V. APPLICATION TO REALISTIC BANDS

To test the scheme for realistic band structures, we have applied it to a number of the metallic elements. The aim was also to give rules for choosing  $W$  and  $N$  in practical applications. Our examples are fcc Al, hcp Zr, and bcc Nb. The energy bands were generated using the standard self-consistent LMTO method.<sup>9</sup> For each case, we have calculated the charge within the Fermi surface and the band energy as a function of the fineness of the uniform  $k$  mesh. The potential and the Fermi energy were kept fixed at the values given by the standard program. Again, the linear tetrahedron method was used for comparison. For each metal, various choices of broadening were tried and one was selected which was characteristic of the range which seemed most suited. One can only give rules of thumb for this choice, since it depends on the shape of the bands in question. The most difficult situations are those in which both steep free-electron-like and flat tight-binding-like bands cross the Fermi surface. For each metal considered, we have chosen a broadening  $W$  such that the first 2–3 approximants are well converged with relatively coarse meshes to their own values, while the next few higher approximants converge absolutely (i.e., to the true value) with the use of a fine mesh. One then has the freedom to choose an  $N$  that will simultaneously optimize the mesh size and the absolute convergence required for the application at hand. For the higher orders (say,  $N > 5$ ) we have found that similar convergence properties can be obtained by taking the next-lower order and a slightly smaller broadening. For the low orders, this is not true: use of  $S_N$  with some low  $N$  gives a gain in precision together with fast  $k$  convergence which cannot be obtained by simply making the zero-order function narrower (as anticipated in Sec. III).

The results obtained with our chosen broadenings are shown in Fig. 5. For the free-electron metal Al, behavior was found which is similar to the low-energy range in the simple-cubic tight-binding band. Because of the wide bands and smooth DOS, a large broadening of 65 mRy could be used. As before, a marked improvement is found if higher-order step functions are used in place of  $S_0$ . For this case, the present scheme is superior to the tetrahedron method.

The situation is qualitatively different for transition metals because of the narrow  $d$  bands. The Fermi surface is more complicated and more  $k$  points are needed to

resolve it properly. The DOS of hcp Zr is very steep at  $E_F$ ; correspondingly, a much smaller broadening of 15 mRy was found suitable. Use of  $S_N$  with  $N=2, 3$ , or 4 then gives quite good convergence for a reasonably small number of  $k$  points. The improvement over the zero-order function is pronounced. The comparison to the linear method shows that the two schemes work about equally well here. Similar conclusions apply to the case of Nb. The band structure at the Fermi energy is still more complicated. Therefore neither method is completely converged for the largest number of  $k$  points we have used. However, in applications such as calculations of frozen-phonon energies it is probably more important to work on a flat part of the curve than to have reached absolute convergence. Then the result is insensitive to the position of the mesh points relative to the Fermi surface and consequently no artificial discontinuities are introduced when the Fermi surface passes over mesh points as the crystal is perturbed. Use of higher step-function approximants makes it possible to reach this flat part and obtain results which are substantially better than with the zero-order function. For the linear method, this kind of convergence cannot be achieved in practice. We have

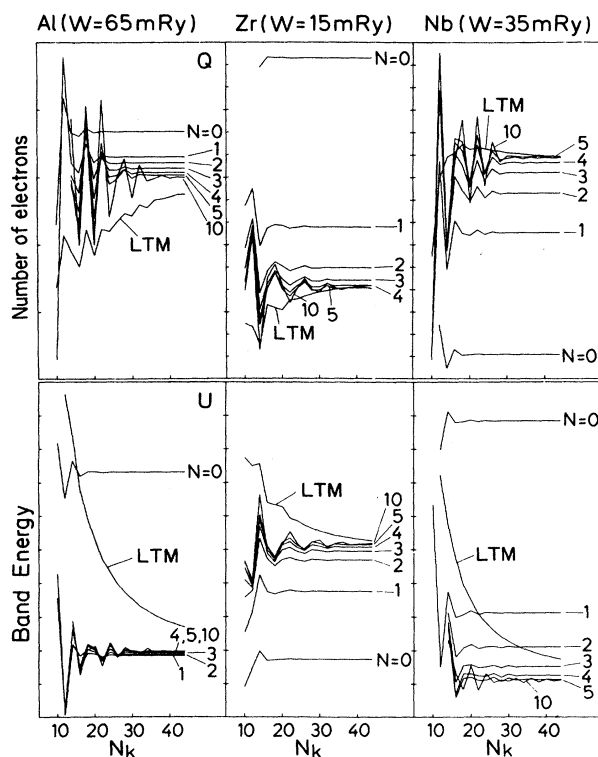


FIG. 5. The  $k$  convergence of the charge  $Q$  and band energy  $U$  at fixed  $E_F$  for the elemental metals Al, Zr, and Nb. Abscissa and labeling of curves as in Fig. 4.  $N_k = 10$  corresponds to 47 irreducible  $k$  points in Al and Nb and to 84 in Zr, while  $N_k = 44$  corresponds to 2168 and 4232, respectively. Spacings between markers on the ordinates are 0.01 electrons for the  $Q$  curves and 1 mRy for the  $U$  curves. Note the expanded scale for the Al  $Q$ .

done similar tests for bcc Mo and paramagnetic bcc Fe. The DOS for Mo has a wide smooth valley near the Fermi energy and a choice of  $W=65$  mRy gives good convergence similar to the Zr results. The case of Fe is similar to Nb and  $W$  near 20 mRy is suitable; both the present approach and the linear tetrahedron method need a very fine mesh to attain absolute convergence here.

The preceding results indicate that two kinds of application are conceivable. For high-precision calculations, it is necessary first to optimize the values of  $W$  and  $N$ , once, for a typical band structure. For this purpose we have found it instructive to make plots of the integrals against the order  $N$  for different finenesses of the mesh and with various fixed broadenings  $W$ . On the other hand, it suffices to be aware in many instances that without any exhaustive testing, an extension of the zero-order smearing method by employing the first- or second-order approximant to  $\delta(x)$  or  $S(x)$  will give a significant enhancement in precision at the expense of minimal extra effort.

## VI. SUMMARY AND CONCLUSIONS

We have introduced a systematic set of smooth approximants to the step and  $\delta$  functions. When convoluted with a given function, these approximants give no error if the function satisfies a well-defined smoothness property. This makes it possible to evaluate Fermi-surface integrals as well as integrals over the occupied part of the Brillouin

zone precisely, using straightforward sampling techniques such as the special-points method. Comparison to results obtained using standard Gaussian smearing show the superiority of the present approach. Tests for realistic metal band structures indicate that the scheme is better suited than the linear tetrahedron method for free-electron metals and about equally successful for transition metals. Our method has advantages common to all sampling schemes, namely (a) all  $\mathbf{k}$  points are treated independently so that it is extremely easy to implement and no large disk files with eigenvalues and eigenvectors are needed, and (b) no errors are introduced by band crossings. The scheme is equally appropriate for  $\mathbf{k}$ -dependent matrix elements as for densities of states and single-particle sums.

It is envisaged that the method may be employed on two levels of complexity. (1) An immediate improvement over standard smearing methods may be obtained, simply by use of the first- or second-order approximants to the step or  $\delta$  function. (2) By careful choice of the parameters  $W$  and  $N$  very high precision in BZ integrations may be achieved which was hitherto unobtainable.

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