

**Note**

**On the Numerical Calculations of the Density of States in Tight-Binding Approximation**

The problem of the calculation of the density of states for the *s*-band and the cubic lattices was solved completely by Jelitto [1]. In the case of the *s*-band the full lattice Green's functions were also calculated (see [2, 3] and references given there). However the half-numerical method of Jelitto and other methods used in the calculations of the lattice Green's functions cannot be used in other cases. For example, in the case of the *d*-band for the simple cubic lattice in the tight-binding approximation, two of five subbands lead to hyperelliptic integrals which cannot be evaluated by the methods similar to that used in [1]. On the other hand, the accuracy of the numerical calculation of the density of states of the previous methods [4, 5] is not sufficient to reproduce the details of the structure of the density of states functions. In the present paper we describe a numerical method of calculating the integrals appearing in the calculations of the densities of states. The method is quite general and was successfully used in the case of the *d*-band [6]. In order to demonstrate the efficiency and the accuracy of the method we have calculated the density of states for the *s*-band in the case of the simple cubic lattice in the tight-binding approximation and compared the results with those given by Jelitto [1].

In the case of the s.c. lattice the density of states can be written in the form [1]:

$$\rho(E) = 8 \int_{-1}^{2-E} dl_1 \int_{-1}^{1-E-l_1} dl_2 I(l_1, l_2) \tag{1}$$

for  $1 \leq E \leq 3$ , and

$$\rho(E) = 8 \left\{ \int_{-1}^{-E} dl_1 \int_{-1-E-l_1}^1 dl_2 I(l_1, l_2) + \int_{-E}^1 dl_1 \int_{-1}^{1-E-l_1} dl_2 I(l_1, l_2) \right\} \tag{2}$$

for  $|E| < 1$ , where

$$I(l_1, l_2) = \{(1 - l_1^2)(1 - l_2^2)[1 - (E + l_1 + l_2)^2]\}^{-1/2}. \tag{3}$$

The direct numerical integration of the double integrals of the type (1) and (2) which does not take into account singularities of the integrand is very slowly convergent and even an accuracy of a few percent can not be practically reached for some values of the parameter *E*.

Introducing new variables:  $l_1 = \sin \varphi_1$ ,  $l_2 = \sin \varphi_2$ , all integrals appearing in Eqs. (1) and (2) can be brought to the form:

$$C(E) = \int_{a_1}^{b_1} d\varphi_1 \int_{a_2}^{b_2} d\varphi_2 Q(\varphi_1, \varphi_2, E) \tag{4}$$

$$\equiv \int_{a_1}^{b_1} d\varphi_1 G(\varphi_1, E),$$

where

$$Q(\varphi_1, \varphi_2, E) = [1 - (E + \sin \varphi_1 + \sin \varphi_2)^2]^{-1/2} \tag{5}$$

and  $G(\varphi_1, E)$  is defined by Eq. (4).

The function  $Q$  as well as the function  $G$  is singular at least at one of the limit of the integral. Both functions  $Q$  and  $G$  can be written in the form:

$$Q(\varphi_1, \varphi_2, E) = p_2(\varphi_2) f_1(\varphi_1, \varphi_2, E), \tag{6}$$

$$G(\varphi_1, E) = p_1(\varphi_1) f_2(\varphi_1, E), \tag{7}$$

where

$$p_i(\varphi_i) = (b_i - \varphi_i)^{\alpha_i} (\varphi_i - a_i)^{\beta_i}, \tag{8}$$

$\alpha_i > -1$ ,  $\beta_i > -1$ .  $a_i$  and  $b_i$  are the lower and the upper limit of the integral, respectively, and  $f_i$  is a regular function on the interval  $[a_i, b_i]$ .

It is well known [7] that the highest order of accuracy of the numerical integration of functions given by Eq. (6) or (7) gives the quadrature:

$$\int_{a_i}^{b_i} p_i(x) f_i(x) dx = \sum_{k=1}^n A_k f_i(x_k), \tag{9}$$

where  $x_k$  are the zeros of the orthogonal polynomials defined by the weight function  $p_i$  on the interval  $[a_i, b_i]$  and  $A_k$  are the coefficients of the quadrature formula.

By a suitable change of variables  $\varphi'_i = c_{i,1}\varphi_i + c_{i,2}$  we can easily extend the intervals of the integration  $[a_i, b_i]$  to  $[-1, 1]$ . We have chosen

$$p_i = (1 - \varphi_i'^2)^{-1/2} \tag{10}$$

for both integrals over  $\varphi'_1$  and  $\varphi'_2$  in Eq. (4). The weight function (10) is not the best weight function for the integrations considered, however it seems to be the best choice from the point of view of the economy of computations. In the case of  $p_i$  given by (10) the orthogonal polynomials are Tchebichef polynomials and zeros of these polynomials are well known ( $x_k = \cos[(2k - 1)\pi/(2n)]$  for  $a_i = -1$  and  $b_i = 1$  in Eq. (9) and for  $p_i(x)$  given by (10), see, for example, [8]). Moreover the coefficients in the quadrature formula assume in this case the constant value ( $A_k = \pi/n$ ).

In the calculations the quadrature (9) with the same number of nodes was used for

TABLE 1  
The Comparison of the Densities of States Obtained by  
Numerical Integration with the Values Given in [1]

$z$	$E = 0$	$E = 1$	$E = 2$
100	70.7893	71.8057	24.0037
150	70.7844	71.950	24.0030
200	70.7826	71.7910	24.0027
400	70.7808	71.7869	24.0025
800	70.7803	71.7858	24.0024
[1]	70.7801 <sup>a</sup>	71.7854	24.0024

<sup>a</sup> There is a missprint in [1]. The correct value for  $E = 0$  is 70.7801 instead of 70.7809 listed in table 1 of the reference 1.

both integrations (over  $\varphi'_1$  and  $\varphi'_2$ ). The results as a function of the number of nodes ( $n$ ) are listed in Table 1. The computations up to  $n = 200$  were performed in single precision, the remaining cases required double precision because the extreme nodes for  $n > 200$  coincide numerically in single precision with the limits of integrations. In all cases the convergence is very good in comparison with methods which do not take into account the end point singularities of integrands. In the case of  $n = 800$  our results differ from those of Jelitto [1] at most on the last (sixth) decimal place.

The remainder for  $n$ -node quadrature can be estimated [7], however the practical use of the formula for the remainder is limited by difficulties in the calculations of the high order derivatives of integrands (particularly in the case of the second integration in the double integral). The convergence of the calculations can be improved by methods for accelerating the convergence [9, 10]. In the simple case of integrals considered here Aitken's  $\Delta^2$  method (based on results for  $n = 100, 200,$  and  $400$ ) gives very good results ( $\rho = 70.7801, 71.7853,$  and  $24.0025$  is obtained for  $E = 0, 1,$  and  $2,$  respectively). In a general case, however, the applicability of this or any other method for accelerating the convergence must be examined.

Convergence acceleration could possibly be achieved with a different choice of weight functions. However, our choice of  $p_i$  is based on the ease with which the nodes and coefficients of the quadrature formula may be calculated.

Although  $p_i$  given by Eq. (10) may not be the best weight function chosen for integrals (4) we hope that the method described can be successfully used not only in the case of the  $d$ -band [6] but also for evaluation of integrals resulting in many other band structure calculation.

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