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# NEW KIND OF PARAMETERIZATION APPLIED TO THE FERMI SURFACE OF A CRYSTALLINE SOLID. PART II: DENSITY OF STATES AND LENGTHS OF ARCS CALCULATED AS A CHECK OF THE THEORY

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**Abstract:** In order to check the validity of parameterization of electron states on the Fermi surface developed in the preceding paper, this parameterization is applied to the calculation of some definite crystal properties. The first property is the density of electron states versus energy in simple cubic and body-centered cubic crystal lattices, examined formerly on the basis of the Bloch parameterization of electron states by Jelitto; the other property is the length of some special arcs extended on the surfaces. The parameterizations of both approaches, that of the present paper and that developed on the basis of the Bloch states, are found to give results remaining in remarkable agreement.

**Keywords:** Fermi surfaces of crystalline solids, electron orbits induced in the magnetic field, density of electron states, orbit lengths and arc lengths on the Fermi surfaces

## 1. Introduction

A difficulty of a conventional description of the Fermi surface done on the basis of the Bloch states is that this kind of parameterization does not make, in general, any reference to the symmetry properties of the mentioned surface. This situation can be changed if a special direction of the Brillouin zone, for example, one of the symmetry axes of that zone, is taken into account (see Part I, [1]). Then all states on the surface lying in a plane normal to the axis can be labeled by the same value of the parameter $a_0$ called the amplitude. The origin of the amplitude notion is connected with the oscillatory behavior of an electron on the Fermi surface when this electron is submitted to the action of a magnetic field directed along the chosen axis of symmetry [2].

In general, the electron states lying on the Fermi surface can be considered as a set of planar parallel orbits which are normal to the applied field. Beyond $a_0$,

the states on a given orbit can be labeled only by a single supplementary variable introduced below as $u$. On the other hand, the parameter $a_0$ is coupled with the Fermi energy with the aid of the wave-vector coordinate $k_z \equiv z$ taken parallel to the chosen axis of symmetry and direction of the field.

This kind of classification of states allowed us, in the first step, to obtain in [1] a better insight into the extremal behavior of some electron observables on the Fermi surface than it could be done before; in the next step, the calculation of the curvature parameters of the surface has been facilitated in a considerable degree.

The aim of the present paper is to check the validity of parameterization developed in [1] by applying it to the crystal properties known from the Bloch's theory. In the first step, the density of electron states versus energy obtained very accurately with the aid of the Bloch's method by Jelitto [3] has been compared, in two crystal cases, with the density of states calculated on the basis of the present method. In the second step, the length of arcs for some special cases of the Fermi surfaces has been considered. The results of both approaches to parameterization of the Fermi surface, that of the present paper and that based on the Bloch states, are found to remain in remarkable agreement.

## 2. The $(u,v)$-parameterization of Fermi surfaces applied in the calculation of the density of states

Taking the tightly-bound s-electrons in the sc lattice as an example our choice of parameterization is:

$$x(u,v) = u, \tag{1}$$

$$y(u,v) = \arccos(1-\cos u+\cos v), \tag{2}$$

where on the basis of (32) and (40) in [1] we have put:

$$v = a_0, \tag{3}$$

and

$$z(u,v) = \arccos(2-E^{\mathrm{sc}}-\cos v) = z(v), \tag{4}$$

on the basis of Equations (29) and (40) in [1]. The limits of the parameters are:

$$0 < u < v \tag{5}$$

for the variable $u$, and

$$0 < v < a_0^{\max} \tag{6}$$

for the variable $v$. The limit of $a_0^{\max}$ in Equation (6) is the value of $a_0$ given in Equation (36) in [1].

In the first step of an approach to the density of states in the sc lattice, we calculate the 1/8 part of the area of the plane $z = \mathrm{const}$ occupied by the electrons. We obtain from Equation (2):

$$S(v) = \int_0^{f(v)} \arccos(1-\cos u+\cos v)du - \frac{1}{2}f^2(v), \tag{7}$$

where $f(v)$ is the function of $v$ calculated from the requirement:

$$\cos x = \cos y. \tag{8}$$

Because of Equations (32) and (40) in [1], we have obtained the following formula for the limit of $u = u^{\lim}$ for the case when Equation (8) is satisfied:

$$2 - 2\cos u^{\lim} = 1 - \cos a_0. \tag{9}$$

In view of Equation (3), Equation (9) gives:

$$f(v) = u^{\lim} = \arccos\left(\frac{1+\cos v}{2}\right). \tag{10}$$

In the next step, $S(v)$ is integrated with the aid of $dz$ equal to:

$$dz = -\frac{\sin v}{[1-(2-E^{\mathrm{sc}}-\cos v)^2]^{1/2}}dv \tag{11}$$

over the interval given in Equation (6) giving 1/16 of $N^{\mathrm{tot}}(E^{\mathrm{sc}})$, the total number of states enclosed within the Fermi surface having the energy $E^{\mathrm{sc}}$. The details of the integration are presented in the Appendix. For the data of the density of states versus energy which is:

$$N(E^{\mathrm{sc}}) = 16\frac{d}{dE^{\mathrm{sc}}}\int_0^{z_{max}} S(v)dz = \frac{dN^{\mathrm{tot}}(E^{\mathrm{sc}})}{dE^{\mathrm{sc}}}, \tag{12}$$

see Table 1.

In the parameterization of the Fermi surface for the bcc lattice is:

$$x(u,v) = u, \tag{13}$$

$$y(u,v) = \arccos\left(\frac{\cos v}{\cos u}\right), \tag{14}$$

$$v = a_0, \tag{15}$$

$$z(u,v) = \arccos\left(\frac{1-E^{\mathrm{bcc}}}{\cos v}\right) = z(v). \tag{16}$$

The limits of the variables $u$ and $v$ entering Equations (13)–(16) can be calculated in a way similar to that applied in the sc case. For the 1/8 part of the area occupied in a plane $z = \mathrm{const}$, we obtain:

$$S(v) = \int_0^{f(v)} \arccos\left(\frac{\cos v}{\cos u}\right)du - \frac{1}{2}f^2(v), \tag{17}$$

where, in view of the assumption (8) taken also for the bcc case:

$$f(v) = u^{\lim} = \arccos(\cos^{1/2} v) \tag{18}$$

on the basis of Equations (33) and (40) of Part I [1]. The function $S(v)$ is integrated next, with the aid of the variable increment $dz$ equal to:

$$dz = -\frac{1-E^{\mathrm{bcc}}}{\left(1-\left(\frac{1-E^{\mathrm{bcc}}}{\cos v}\right)^2\right)^{1/2}}\frac{\sin v}{\cos^2 v}dv, \tag{19}$$

over the interval of $v$ equal to (6), in which $a_0^{\max}$ is defined again by Equation (30) in [1]. The density of states in the bcc lattice versus energy done with the aid of parameterization given in Equations (13)–(16) is presented in Table 2 (some details of the calculations are given in the Appendix).

**Table 1.** Density of the tightly-bound $s$-electron states in the sc lattice calculated with the aid of $(u,v)$-parameterization of the electron orbits for different energies $E^{\mathrm{sc}}$. Only the closed orbits within the interval $0 < E^{\mathrm{sc}} < 2$ are considered. The data are compared with the density of states obtained by Jelitto [3] on the basis of a conventional Bloch parameterization of the Fermi surfaces

| $E^{\mathrm{sc}}$ | density by the present theory | density by Jelitto | ratio of column 3 and column 2 | $E^{\mathrm{sc}}$ | density by the present theory | density by Jelitto | ratio of column 3 and column 2 |
|---|---|---|---|---|---|---|---|
| 0.01 | 1.7816 | 1.7816 | 1.0000 | 1.05 | 25.0617 | 25.0617 | 1.0000 |
| 0.02 | 2.5259 | 2.5259 | 1.0000 | 1.1 | 26.1521 | 26.1521 | 1.0000 |
| 0.03 | 3.1014 | 3.1014 | 1.0000 | 1.15 | 27.2777 | 27.2777 | 1.0000 |
| 0.04 | 3.5902 | 3.5902 | 1.0000 | 1.2 | 28.4428 | 28.4428 | 1.0000 |
| 0.05 | 4.0242 | 4.0242 | 1.0000 | 1.25 | 29.6524 | 29.6524 | 1.0000 |
| 0.1 | 5.7643 | 5.7643 | 1.0000 | 1.3 | 30.9120 | 30.9120 | 1.0000 |
| 0.15 | 7.1521 | 7.1521 | 1.0000 | 1.35 | 32.2282 | 32.2281 | 1.0000 |
| 0.2 | 8.3683 | 8.3683 | 1.0000 | 1.4 | 33.6085 | 33.6085 | 1.0000 |
| 0.25 | 9.4825 | 9.4825 | 1.0000 | 1.45 | 35.0621 | 35.0621 | 1.0000 |
| 0.3 | 10.5302 | 10.5302 | 1.0000 | 1.5 | 36.6000 | 36.6000 | 1.0000 |
| 0.35 | 11.5330 | 11.5329 | 1.0000 | 1.55 | 38.2360 | 38.2360 | 1.0000 |
| 0.4 | 12.5047 | 12.5047 | 1.0000 | 1.6 | 39.9876 | 39.9876 | 1.0000 |
| 0.45 | 13.4554 | 13.4554 | 1.0000 | 1.65 | 41.8777 | 41.8776 | 1.0000 |
| 0.5 | 14.3926 | 14.3926 | 1.0000 | 1.7 | 43.9374 | 43.9373 | 1.0000 |
| 0.55 | 15.3223 | 15.3223 | 1.0000 | 1.75 | 46.2112 | 46.2112 | 1.0000 |
| 0.6 | 16.2493 | 16.2493 | 1.0000 | 1.8 | 48.7670 | 48.7669 | 1.0000 |
| 0.65 | 17.1778 | 17.1778 | 1.0000 | 1.85 | 51.7176 | 51.7175 | 1.0000 |
| 0.7 | 18.1114 | 18.1114 | 1.0000 | 1.9 | 55.2820 | 55.2819 | 1.0000 |
| 0.75 | 19.0538 | 19.0537 | 1.0000 | 1.95 | 60.0209 | 60.0208 | 1.0000 |
| 0.8 | 20.0076 | 20.0076 | 1.0000 | 1.96 | 61.2437 | 61.2436 | 1.0000 |
| 0.85 | 20.9764 | 20.9764 | 1.0000 | 1.97 | 62.6382 | 62.6381 | 1.0000 |
| 0.9 | 21.9630 | 21.9630 | 1.0000 | 1.98 | 64.3008 | 64.3007 | 1.0000 |
| 0.95 | 22.9706 | 22.9706 | 1.0000 | 1.99 | 66.4796 | 66.4795 | 1.0000 |
| 1.0 | 24.0024 | 24.0024 | 1.0000 | | | | |

## 3. Arc lengths and orbit lengths lying on the Fermi surface

Some arcs on the Fermi surface, for example, those lying in a plane parallel to the magnetic field and containing axis $z$ cannot be classified as those belonging to $u = \mathrm{const}$ or $v = \mathrm{const}$. Calculations for such arcs require, in general, a rather complicated formula for the arc element, *viz.* [4, 5]:

$$ds = (Edu^2 + 2Fdudv + Gdv^2)^{1/2}, \tag{20}$$

where

$$E = \left(\frac{\partial \vec{r}}{\partial u}\right)^2, \quad F = \frac{\partial \vec{r}}{\partial u} \cdot \frac{\partial \vec{r}}{\partial v}, \quad G = \left(\frac{\partial \vec{r}}{\partial v}\right)^2, \tag{21}$$

and $\vec{r}$ is a position vector having the coordinates $x = x(u,v)$, $y = y(u,v)$, $z = z(u,v)$. This complication can be avoided by combining the equation for the electron energy with that for a plane in which the arc is located. In the first step, we consider a plane

$$y = 0, \tag{22}$$

equivalent to the plane $x = 0$ by symmetry, which contains both the axis $z$ parallel to the magnetic field and the examined arc.

**Table 2.** Density of the tightly-bound $s$-electron states in the bcc lattice calculated with the aid of $(u,v)$-parameterization of the electron orbits for different energies $E^{\mathrm{bcc}}$. Only the closed orbits within the interval $0 < E^{\mathrm{bcc}} < 1$ are considered. The data are compared with those obtained by Jelitto [3] on the basis of conventional Bloch parameterization of the Fermi surfaces

| $E^{\mathrm{bcc}}$ | density by the present theory | density by Jelitto | ratio of column 3 and column 2 | $E^{\mathrm{bcc}}$ | density by the present theory | density by Jelitto | ratio of column 3 and column 2 |
|---|---|---|---|---|---|---|---|
| 0.001 | 4.4992 | 4.4992 | 1.0000 | 0.60 | 206.478 | 206.478 | 1.0000 |
| 0.006 | 11.0624 | 11.0624 | 1.0000 | 0.65 | 233.304 | 233.304 | 1.0000 |
| 0.011 | 15.0352 | 15.0352 | 1.0000 | 0.70 | 265.440 | 265.439 | 1.0000 |
| 0.016 | 18.2021 | 18.2020 | 1.0000 | 0.75 | 305.180 | 305.179 | 1.0000 |
| 0.021 | 20.9326 | 20.9326 | 1.0000 | 0.80 | 356.502 | 356.502 | 1.0000 |
| 0.03 | 25.1924 | 25.1923 | 1.0000 | 0.85 | 427.188 | 427.187 | 1.0000 |
| 0.04 | 29.3150 | 29.3150 | 1.0000 | 0.90 | 535.656 | 535.655 | 1.0000 |
| 0.05 | 33.0314 | 33.0313 | 1.0000 | 0.91 | 565.552 | 565.551 | 1.0000 |
| 0.06 | 36.4692 | 36.4692 | 1.0000 | 0.92 | 599.812 | 599.811 | 1.0000 |
| 0.07 | 39.7044 | 39.7045 | 1.0000 | 0.93 | 639.726 | 639.725 | 1.0000 |
| 0.08 | 42.7864 | 42.7863 | 1.0000 | 0.94 | 687.222 | 687.220 | 1.0000 |
| 0.09 | 45.7490 | 45.7489 | 1.0000 | 0.95 | 745.360 | 745.359 | 1.0000 |
| 0.10 | 48.6174 | 48.6173 | 1.0000 | 0.955 | 779.928 | 779.927 | 1.0000 |
| 0.15 | 62.0846 | 62.0846 | 1.0000 | 0.96 | 819.414 | 819.413 | 1.0000 |
| 0.20 | 74.9000 | 74.8999 | 1.0000 | 0.965 | 865.256 | 865.253 | 1.0000 |
| 0.25 | 87.6892 | 87.6892 | 1.0000 | 0.97 | 919.594 | 919.592 | 1.0000 |
| 0.30 | 100.843 | 100.843 | 1.0000 | 0.975 | 985.830 | 985.827 | 1.0000 |
| 0.35 | 114.676 | 114.676 | 1.0000 | 0.98 | 1069.79 | 1069.79 | 1.0000 |
| 0.40 | 129.491 | 129.491 | 1.0000 | 0.985 | 1182.75 | 1182.74 | 1.0000 |
| 0.45 | 145.620 | 145.620 | 1.0000 | 0.99 | 1350.94 | 1350.94 | 1.0000 |
| 0.50 | 163.460 | 163.460 | 1.0000 | 0.995 | 1662.85 | 1662.84 | 1.0000 |
| 0.55 | 183.518 | 183.518 | 1.0000 | | | | |

In the first step, the property (22) transforms the energy expression in the sc lattice (see Equation (41) in [1]) into:

$$E^{\mathrm{sc}} = 2 - \cos x - \cos z \tag{23}$$

which gives the derivative:

$$\frac{dz}{dx} = -\frac{\sin x}{\sin z} = -\frac{\sin x}{(1-(2-E^{\mathrm{sc}}-\cos x)^2)^{1/2}}. \tag{24}$$

This result can be substituted to the integral for 1/4-th of the arc length:

$$\frac{1}{4}L_{\parallel}^{\mathrm{latt}} = \int_0^{x^{\max}} \left(1+\left(\frac{dz}{dx}\right)^2\right)^{1/2} dx \tag{25}$$

extended between $x = 0$ and

$$x^{\max} = a_0^{\max}. \tag{26}$$

The parameter $a_0^{\max}$ is coupled with $E^{\mathrm{sc}}$, expressed for $z = 0$ by the formula:

$$E^{\mathrm{sc}} = 1 - \cos a_0^{\max}, \tag{27}$$

valid also for the case of $y=0$. In Table 3 we present the dependence of $L_{\|}^{\mathrm{sc}}$ on $E^{\mathrm{sc}}$, as well as the convergence of $L_{\|}^{\mathrm{sc}}$ to its limiting value attained in effect of an approach of $E^{\mathrm{sc}}$ to:

$$E^{\mathrm{sc}}=2 \tag{28}$$

which is the upper limit of energy for the closed electron orbits obtained in the $(x,y)$ plane [2].

**Table 3.** Lengths of arcs $L_{\|}^{\mathrm{sc}}$ and orbit lengths $L_{\perp}^{\mathrm{sc}}$ on the Fermi surface of the sc lattice, calculated as functions of the energy, $E^{\mathrm{sc}}$, of the tightly-bound $s$-electrons. The $L_{\|}^{\mathrm{sc}}$ are in a plane parallel to the axis $z$ ($y=0$ or $x=0$); the $L_{\perp}^{\mathrm{sc}}$ are calculated in a plane normal to the magnetic field ($z=0$). Only the interval of energy corresponding to closed orbits is considered in the calculations. The maximal values of $(1/4)L_{\|}^{\mathrm{sc}}$ and $(1/4)L_{\perp}^{\mathrm{sc}}$ tend to the value equal to $\sqrt{2}\pi$ calculated from the geometry of the Brillouin zone (see Equation (31) and inferences below Equation (51)). The length of the edge of the Brillouin zone is assumed as equal to $\pi$

| $E^{\mathrm{sc}}$ | $(1/4)L_{\|}^{\mathrm{sc}}$ | $(1/4)L_{\perp}^{\mathrm{sc}}$ | $E^{\mathrm{sc}}$ | $(1/4)L_{\|}^{\mathrm{sc}}$ | $(1/4)L_{\perp}^{\mathrm{sc}}$ |
|---|---|---|---|---|---|
| 0.2 | 1.0064 | 1.0064 | 1.94 | 4.0232 | 4.0233 |
| 0.4 | 1.4433 | 1.4433 | 1.95 | 4.0605 | 4.0605 |
| 0.6 | 1.7948 | 1.7949 | 1.96 | 4.1015 | 4.1015 |
| 0.8 | 2.1077 | 2.1077 | 1.97 | 4.1478 | 4.1478 |
| 1.0 | 2.4014 | 2.4014 | 1.98 | 4.2024 | 4.2024 |
| 1.2 | 2.6883 | 2.6883 | 1.99 | 4.2731 | 4.2731 |
| 1.4 | 2.9796 | 2.9797 | 1.9998 | 4.4189 | 4.4189 |
| 1.6 | 3.2910 | 3.2910 | 1.99985 | 4.4221 | 4.4221 |
| 1.8 | 3.6571 | 3.6572 | 1.9999 | 4.4259 | 4.4259 |
| 1.9 | 3.8972 | 3.8973 | 1.99995 | 4.4309 | 4.4309 |
| 1.91 | 3.9261 | 3.8973 | 1.99997 | 4.4336 | 4.4336 |
| 1.92 | 3.9566 | 3.9566 | 1.99999 | 4.4375 | 4.4375 |
| 1.93 | 3.9888 | 3.9888 | 1.999998 | 4.4405 | 4.4405 |

The length of arc (25) for this limiting case can also be estimated from the conventional theory of the Brillouin zones [6, 7], because the arc $(1/4)(L_{\|}^{\mathrm{sc}})^{\max}$ on the plane $y=0$, or $x=0$, is a straight line, going from one of the points:

$$(\pm\pi,0,0), \qquad (0,\pm\pi,0) \tag{29}$$

lying on the plane $z=0$ to one of the points:

$$(0,0,\pm\pi) \tag{30}$$

lying on the boundary of the zone, being a plane $z=\pi$ or $z=-\pi$. The length of $(1/4)(L_{\|}^{\mathrm{sc}})^{\max}$ is therefore:

$$\frac{1}{4}(L_{\|}^{\mathrm{sc}})^{\max}=[(0-0)^2+(\pi-0)^2+(\pi-0)^2]^{1/2}=\sqrt{2}\pi\cong 4.44, \tag{31}$$

the result which is close to that calculated for $(1/4)L_{\|}^{\mathrm{sc}}$ in Table 3.

An arc length $L_{\|}^{\mathrm{bcc}}$ can be considered also for the Fermi surface in the bcc lattice. The case of $y=0$ gives (see Equation (66) in [1]):

$$E^{\mathrm{bcc}}=1-\cos x\cos z \tag{32}$$

which leads to:

$$\frac{dz}{dx} = -\frac{\sin x \cos z}{\sin z \cos x} = -\frac{\sin x \left(\frac{1-E^{\mathrm{bcc}}}{\cos x}\right)}{\left(1-\left(\frac{1-E^{\mathrm{bcc}}}{\cos x}\right)^2\right)^{1/2} \cos x}. \tag{33}$$

The upper limit of the integral (25) is given by the plane $z=0$, so (see Equation (30) in [1]):

$$x^{\max} = a_0^{\max} = \arccos(1-E^{\mathrm{bcc}}). \tag{34}$$

A substitution of Equation (33) for $dz/dx$ under the integral in Equation (25) gives $L_{\parallel}^{\mathrm{bcc}}$ as a function of $E^{\mathrm{bcc}}$. A maximum value of $L_{\parallel}^{\mathrm{bcc}}$ corresponds to the energy:

$$E^{\mathrm{bcc}} = 1 \tag{35}$$

for which maximal closed orbits for the bcc lattice in the planes $z=\mathrm{const}$ are also obtained [2].

In this limiting case of the electron energy, *viz.* Equation (35), the arc length $(1/4)(L_{\parallel}^{\mathrm{bcc}})^{\max}$ can be calculated directly from an examination of the Brillouin zone [8]. The arc begins, for example, in one of the points:

$$(\pm\pi/2,0,0), \quad \text{or} \quad (0,\pm\pi/2,0), \tag{36}$$

lying on the plane $z=0$ of the zone. Going next across one of the points:

$$(\pm\pi/2,0,\pm\pi/2), \quad \text{or} \quad (0,\pm\pi/2,\pm\pi/2), \tag{37}$$

having the $(x,y)$ coordinates the same as in Equation (36), the end point of the arc $(1/4)(L_{\parallel}^{\mathrm{bcc}})^{\max}$ is at one of the points:

$$(0,\pm\pi/2,\pm\pi/2), \quad \text{or} \quad (\pm\pi/2,0,\pm\pi/2), \tag{38}$$

in which the $z$-coordinate considered in Equation (37) remains unchanged. In effect, the length $(1/4)(L_{\parallel}^{\mathrm{bcc}})^{\max}$ becomes:

$$\frac{1}{4}(L_{\parallel}^{\mathrm{bcc}})^{\max} = \pi/2+\pi/2 = \pi. \tag{39}$$

A dependence of the length $(1/4)L_{\parallel}^{\mathrm{bcc}}$ calculated from Equations (25) and (33) on $E^{\mathrm{bcc}}$, and the convergence of this length to the limiting number given in Equation (39) are presented in Table 4.

The orbit lengths, extended along the cross-sections of the Fermi surface with the planes $z=\mathrm{const}$, can be also easily calculated. For free electrons we have the relations obtained from those for the crystal electron cases (see Equations (32)–(34) in [1]) at small $x$, $y$ and $z$:

$$a_0^2 = x^2+y^2, \tag{40}$$

hence

$$2E^{\mathrm{free}} = a_0^2+z^2 \tag{41}$$

(see Equations (18) and (40) in [1]). The length of the circumference of a circle represented by the Equation (40) is:

$$L_{\perp}^{\mathrm{free}} = 2\pi a_0 \tag{42}$$

being proportional to the number of states lying on that circumference.

**Table 4.** Lengths of arcs $L_{\parallel}^{\mathrm{bcc}}$ and orbit lengths $L_{\perp}^{\mathrm{bcc}}$ on the Fermi surface of the bcc lattice calculated as functions of energy $E^{\mathrm{bcc}}$ of the tightly-bound $s$-electrons. Only the interval of energy corresponding to the closed orbits is examined. The $L_{\parallel}^{\mathrm{bcc}}$ are lying in a plane $y=0$ (equivalent to $x=0$ by symmetry) containing the axis $z$; the $L_{\perp}^{\mathrm{bcc}}$ are in a plane $z=0$ normal to the magnetic field. The maximum values of $(1/4)L_{\parallel}^{\mathrm{bcc}}$ and $(1/4)L_{\perp}^{\mathrm{bcc}}$ tend to the value equal to $\pi$ calculated from the geometry of the Brillouin zone (see Equations (39) and (60)). The length of the edge of the zone is assumed equal to $(1/2)\sqrt{3}\pi$

| $E^{\mathrm{bcc}}$ | $(1/4)L_{\parallel}^{\mathrm{bcc}}$ | $(1/4)L_{\perp}^{\mathrm{bcc}}$ | $E^{\mathrm{bcc}}$ | $(1/4)L_{\parallel}^{\mathrm{bcc}}$ | $(1/4)L_{\perp}^{\mathrm{bcc}}$ |
|---|---|---|---|---|---|
| 0.1 | 0.7116 | 0.7116 | 0.96 | 2.7975 | 2.7978 |
| 0.2 | 1.0206 | 1.0206 | 0.97 | 2.8446 | 2.8449 |
| 0.3 | 1.2691 | 1.2692 | 0.98 | 2.8998 | 2.9002 |
| 0.4 | 1.4903 | 1.4904 | 0.99 | 2.9710 | 2.9715 |
| 0.5 | 1.6980 | 1.6981 | 0.9991 | 3.0907 | 3.0907 |
| 0.6 | 1.9009 | 1.9009 | 0.9992 | 3.0937 | 3.0937 |
| 0.7 | 2.1069 | 2.1069 | 0.9993 | 3.0968 | 3.0968 |
| 0.8 | 2.3270 | 2.3271 | 0.9994 | 3.1001 | 3.1001 |
| 0.9 | 2.5859 | 2.5860 | 0.9995 | 3.1037 | 3.1037 |
| 0.91 | 2.6163 | 2.6164 | 0.9996 | 3.1077 | 3.1077 |
| 0.92 | 2.6481 | 2.6483 | 0.9997 | 3.1122 | 3.1122 |
| 0.93 | 2.6816 | 2.6818 | 0.9998 | 3.1176 | 3.1176 |
| 0.94 | 2.7172 | 2.7174 | 0.9999 | 3.1246 | 3.1247 |
| 0.95 | 2.7555 | 2.7558 | 0.99999 | 3.1362 | 3.1362 |

The method of calculating the orbit length in a crystal case is similar to that applied before for the arcs. For the sc lattice, taken as an example, we have:

$$1-\cos a_0 = 2-\cos x-\cos y \tag{43}$$

hence, for a constant $a_0$,

$$\sin x\,dx+\sin y\,dy=0 \tag{44}$$

or

$$\frac{dy}{dx}=-\frac{\sin x}{\sin y}. \tag{45}$$

This provides us with one-fourth of the orbit length $L_{\perp}^{\mathrm{sc}}$ calculated at some value of $a_0$:

$$\begin{aligned}\frac{1}{4}L_{\perp}^{\mathrm{sc}} &= \int_0^{a_0}\sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx = \int_0^{a_0}\frac{[1-(1-\cos x+\cos a_0)^2+\sin^2 x]^{1/2}}{[1-(1-\cos x+\cos a_0)^2]^{1/2}}dx \\ &= 2\int_0^{f(a_0)}\frac{[1-(1-\cos x+\cos a_0)^2+\sin^2 x]^{1/2}}{[1-(1-\cos x+\cos a_0)^2]^{1/2}}dx\end{aligned} \tag{46}$$

on condition that the relation between $x$ and $y$ given in (43) is taken into account. In order to avoid the divergence of the integrand at the limit of $x=a_0$, the integral limit in Equation (46) has been changed, in the second step, to that attained at $x=y$; because of Equation (43) (see also Equations (8) and (10)), we obtain for this limit:

$$f(a_0)=\arccos\left(\frac{1+\cos a_0}{2}\right). \tag{47}$$

The length $L_{\perp}^{\mathrm{sc}}$ can be made dependent on $z$ if we note that $a_0$ and $z$ are coupled by the formula (see Equations (29) and (40) in [1]):

$$E^{\mathrm{sc}}=2-\cos a_0-\cos z. \tag{48}$$

The variable $z$ is covering the interval:

$$-\arccos(1-E^{\mathrm{sc}}) < z < \arccos(1-E^{\mathrm{sc}}) \tag{49}$$

(see Equations (38) and (40) in [1]). The limits in Equation (49) correspond to a situation when $a_0$ is decreased to its zero value, a maximum of $a_0$ for a given $E^{\mathrm{sc}}$ can be attained at $z=0$ and is corresponding to the relation:

$$E^{\mathrm{sc}} = 1-\cos a_0 \tag{50}$$

(see Equation (48)).

In the next step, a maximal closed orbit on the plane $z=0$ can be obtained at $E^{\mathrm{sc}}=2$, so $a_0=\pi$ in this case [2], and the orbit itself is a square on the plane $z=0$ of the Brillouin zone extended between the points:

$$(0,\pi,0), \quad (\pi,0,0), \quad (0,-\pi,0), \quad (-\pi,0,0) \tag{51}$$

each lying on the boundary of the Brillouin zone (the length of the lattice parameter is assumed equal to a unit distance, therefore the square has the edge equal to $2^{1/2}\pi$). The dependence of $(1/4)L_{\perp}^{\mathrm{sc}}$ on $E^{\mathrm{sc}}$ is presented in Table 3, the maximum of $(1/4)L_{\perp}^{\mathrm{sc}}$ is equal to $(1/4)(L_{\parallel}^{\mathrm{sc}})^{\max}$ calculated in Equation (30) (see Table 3).

For the bcc lattice, we have:

$$E^{\mathrm{bcc}} = 1-\cos a_0 \cos z \tag{52}$$

and

$$\cos a_0 = \cos x \cos y, \tag{53}$$

so a constant $a_0$ gives

$$-\sin x \cos y\, dx - \cos x \sin y\, dy = 0 \tag{54}$$

or

$$\frac{dy}{dx} = -\frac{\sin x \cos y}{\cos x \sin y}. \tag{55}$$

The formula for one-fourth of the orbit length having the amplitude $a_0$ is:

$$\begin{aligned}\frac{1}{4}L_{\perp}^{\mathrm{bcc}} &= \int_0^{a_0}\sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx = \int_0^{a_0}\left(1+\frac{\sin^2 x\cos^2 y}{\cos^2 x \sin^2 y}\right)^{1/2}dx \\ &= \int_0^{a_0}\left(1+\frac{\sin^2 x\cos^2 a_0}{\cos^2 x(\cos^2 x-\cos^2 a_0)}\right)^{1/2}dx \\ &= 2\int_0^{f(a_0)}\left(1+\frac{\sin^2 x\cos^2 a_0}{\cos^2 x(\cos^2 x-\cos^2 a_0)}\right)^{1/2}dx.\end{aligned} \tag{56}$$

In the calculation of (56) the relations (52) and (18) for $v=a_0$ have been taken into account; the last step in Equation (56) makes it possible to avoid the divergence of the integrand at $x=a_0$. Expression (56) is a $z$-dependent quantity if we note that variable $z$ is coupled with $a_0$ on the basis of (52). The interval of $z$ is extended between the limits:

$$-\arccos(1-E^{\mathrm{bcc}}) < z < \arccos(1-E^{\mathrm{bcc}}) \tag{57}$$

obtained from Equations (38) and (40) in [1].

A maximum of $a_0$ for a given $E^{\mathrm{bcc}}$ is obtained at $z=0$ and satisfies the relation:

$$E^{\mathrm{bcc}} = 1 - \cos a_0 \tag{58}$$

(see Equations (52) and (34)). A maximal closed orbit on the plane $z=0$ has:

$$a_0 = \pi/2, \tag{59}$$

because $E^{\mathrm{bcc}} = 1$ in this case. The orbit has then the shape of a square with edges equal to $\pi$, and the corners of the square have the coordinates:

$$(-\pi/2,\pi/2,0), \quad (\pi/2,\pi/2,0), \quad (\pi/2,-\pi/2,0), \quad (-\pi/2,-\pi/2,0) \tag{60}$$

touching the boundary of the Brillouin zone in the plane $z=0$ (see [8]). This implies that $(1/4)(L_{\perp}^{\mathrm{bcc}})^{\max}$ is equal to $\pi$ (*cf.* here Equation (39)). For the dependence of $(1/4)L_{\perp}^{\mathrm{bcc}}$ on $E^{\mathrm{bcc}}$ see Table 4.

## 4. The validity of $(u,v)$-parameterization tested in the examination of a spherical Fermi surface

The validity of the $(u,v)$-parameterization in the examination of the Fermi surface can be checked also in the case of free electrons. In the first step, let us note that for small $E^{\mathrm{latt}}$, the electron energy on the Fermi surface tends to:

$$E^{\mathrm{free}} = \mathrm{const} \tag{61}$$

(see Equation (18) in [1]). By taking small $a_0$ and small $z$, the electron energy in any cubic lattice becomes:

$$E^{\mathrm{free}} = \frac{a_0^2}{2} + \frac{z^2}{2}. \tag{62}$$

In the same conditions, a coupling between $x$, $y$ and $a_0$ is represented by the formula (40). A substitution of (40) into (62) provides us with the expression for:

$$E^{\mathrm{free}} = \frac{x^2}{2} + \frac{y^2}{2} + \frac{z^2}{2} \tag{63}$$

equal to that given in Equation (18) in [1] (see also Equation (40) in [1]).

In the procedure of parameterization of the surface (61), we can use the same variables $(u,v)$ as in the case of the Fermi surface of the crystal electrons:

$$x = x_s(u,v) = u, \tag{64}$$

$$v = a_0, \tag{65}$$

but here

$$y = y_s(u,v) = (a_0^2 - u^2)^{1/2} = (v^2 - u^2)^{1/2}. \tag{66}$$

Simultaneously, because of Equations (62) and (65), we have:

$$z = z_s(u,v) = (2E^{\mathrm{free}} - v^2)^{1/2} \tag{67}$$

which is solely a function of the variable $v$. Our test is limited to the arc-length parameters (21) entering (20). We have:

$$E_s = \left(\frac{\partial x_s}{\partial u}\right)^2 + \left(\frac{\partial y_s}{\partial u}\right)^2 + \left(\frac{\partial z_s}{\partial u}\right)^2 = 1 + \frac{u^2}{v^2 - u^2}, \tag{68}$$

$$F_s = \frac{\partial x_s}{\partial u}\frac{\partial x_s}{\partial v} + \frac{\partial y_s}{\partial u}\frac{\partial y_s}{\partial v} + \frac{\partial z_s}{\partial u}\frac{\partial z_s}{\partial v} = -\frac{uv}{v^2-u^2}, \tag{69}$$

$$G_s = \left(\frac{\partial x_s}{\partial v}\right)^2 + \left(\frac{\partial y_s}{\partial v}\right)^2 + \left(\frac{\partial z_s}{\partial v}\right)^2 = \frac{v^2}{v^2-u^2} + \frac{v^2}{2E^{\text{free}}-v^2}. \tag{70}$$

Half of the length of the arc along the $u$-curve ($v = \text{const}$) can be calculated from the formula:

$$\begin{aligned}\int_{-a_0}^{a_0} \sqrt{E_s}du &= \int_{-a_0}^{a_0} \frac{v du}{(v^2-u^2)^{1/2}} \\ &= a_0 \int_{-a_0}^{a_0} \frac{du}{(a_0^2-u^2)^{1/2}} = a_0 \arcsin\left(\frac{u}{a_0}\right)\Big|_{u=-a_0}^{u=a_0} = \pi a_0,\end{aligned} \tag{71}$$

obtained on the basis of Equation (68) and the relation (65). This provides us with an expected orbit length on a free-electron Fermi surface (see Equation (42)).

One-fourth of the length of the arc lying in a plane containing the $z$-axis parallel to the magnetic field can be calculated by referring to the expression for the electron energy. Taking, for example, the case of $y = 0$, we have:

$$2E^{\text{free}} = x^2 + z^2, \tag{72}$$

from which

$$0 = x\,dx + z\,dz, \tag{73}$$

so

$$\frac{dz}{dx} = -\frac{x}{z}, \qquad \frac{dy}{dx} = 0, \tag{74}$$

and

$$\begin{aligned}\frac{1}{4}L_{\|} &= \int_0^{\sqrt{2E^{\text{free}}}} \left(1+\frac{x^2}{z^2}\right)^{1/2} dx \\ &= (2E^{\text{free}})^{1/2} \int_0^{\sqrt{2E^{\text{free}}}} \frac{dx}{\sqrt{2E^{\text{free}}-x^2}} = (2E^{\text{free}})^{1/2} \arcsin 1 = \frac{\pi}{2}(2E^{\text{free}})^{1/2}\end{aligned} \tag{75}$$

provides us with an expected result for 1/4 of the arc length on a spherical surface. The upper limit of the integral (75) is that obtained from (72) at $z = 0$.

An area of the parameterised Fermi surface can be obtained by choosing 1/8 of the whole area for the calculations. From Equations (68)–(70) we have:

$$(E_s G_s - F_s^2)^{1/2} = \frac{(2E^{\text{free}})^{1/2} v}{(v^2-u^2)^{1/2}(2E^{\text{free}}-v^2)^{1/2}}. \tag{76}$$

This gives:

$$\begin{aligned}\int_0^{a_0^{\max}} dv \int_0^v du &= (2E^{\text{free}})^{1/2} \int_0^{a_0^{\max}} \frac{v\,dv}{(2E^{\text{free}}-v^2)^{1/2}} \int_0^v \frac{du}{(v^2-u^2)^{1/2}} \\ &= (2E^{\text{free}})^{1/2} \frac{\pi}{2} \int_0^{a_0^{\max}} dv \frac{v}{(2E^{\text{free}}-v^2)^{1/2}} \\ &= -(2E^{\text{free}})^{1/2} \frac{\pi}{2} (2E^{\text{free}}-v^2)^{1/2}\Big|_{v=0}^{v=a_0^{\max}} = \pi E^{\text{free}}\end{aligned} \tag{77}$$

which is 1/8 of the surface of a sphere having radius $(2E^{\text{free}})^{1/2}$. The case of $a_0^{\max} = (2E^{\text{free}})^{1/2}$ is attained at $z = 0$ (see Equation (62)).

## 5. Summary

The properties of three-dimensional Fermi surfaces are found to be much easier to examine when the idea of symmetry, due – for example – to the presence of an external magnetic field acting along one of the crystallographic symmetry axes, is applied. This facility is due mainly to parameterization properties of the electron states when the effect of symmetry is taken into account. In particular, the states lying in the same plane of the reciprocal space normal to the symmetry axis are coupled together, forming an orbit on the Fermi surface characteristic for each plane. Since the positions of the planes can change continuously along the field, the orbits cover the whole of the Fermi surface.

The accuracy of the new kind of parameterization of the electron states is illustrated for the Fermi surfaces of the tightly-bound *s*-electrons in cubic crystal lattices taken as examples.

In the first step, the validity of parameterization developed in the former paper (Part I) is checked in train of calculations of the density of states versus the electron energy. These calculations of the Fermi surface done on the basis of the Bloch parameterization by Jelitto are compared with the density of states obtained from the present method.

In the second step, the special arc lengths on the Fermi surface – easily obtainable from the Bloch theory – are compared with an estimate of the lengths of arcs done with the aid of the present formalism. The agreement of the data calculated in the framework of both kinds of the applied parameterizations, Bloch's and the present one, is remarkable.

## Appendix. Integrals needed for calculation of the density of states in the sc and bcc crystal lattices

The number of states in a crystal lattice is proportional to the volume enclosed by the Fermi surface:

$$E^{\mathrm{latt}}(x,y,z) = \mathrm{const.} \tag{A1}$$

This surface, in the case of the sc lattice, is expressed by the formula (41) in [1]. If we use the parameterization (1)–(4), we can present this volume as follows:

$$N^{\mathrm{tot}}(E^{\mathrm{sc}}) = 16 \int_0^{z_{max}} dz \left( \int_0^{f(v)} \arccos(1+\cos v-\cos u)du - \frac{1}{2}f^2(v) \right). \tag{A2}$$

With the aid of Equation (10), the volume (A2) can be represented by the expression:

$$N^{\mathrm{tot}}(E^{\mathrm{sc}}) = 8 \int_0^{z_{max}} dz \times \left( 2 \int_0^{\arccos\left(\frac{1+\cos v}{2}\right)} \arccos(1+\cos v-\cos u)du - \left(\arccos\left(\frac{1+\cos v}{2}\right)\right)^2 \right). \tag{A3}$$

In the next step, the right-hand side of Equation (A3) refers to $E^{\mathrm{sc}}$ explicitly. Because of Equations (38), (40) in [1] and Equation (11), the formula (A3) is transformed into:

$$N^{\mathrm{tot}}(E^{\mathrm{sc}}) = 8 \int_0^{\arccos(1-E^{\mathrm{sc}})} \frac{\sin v\, dv}{[1-(2-E^{\mathrm{sc}}-\cos v)^2]^{1/2}} \times \left( 2 \int_0^{\arccos\left(\frac{1+\cos v}{2}\right)} \arccos(1+\cos v-\cos u)du - \left(\arccos\left(\frac{1+\cos v}{2}\right)\right)^2 \right). \tag{A4}$$

A simplification of (A4) is obtained by a substitution:

$$\cos v = 1 - E_\perp \tag{A5}$$

where $E_\perp$ is a part of the electron energy depending solely on $x$ and $y$. This leads to:

$$dE_\perp = \sin v\, dv \tag{A6}$$

and

$$N^{\mathrm{tot}}(E^{\mathrm{sc}}) = 8 \int_0^{E^{\mathrm{sc}}} \frac{dE_\perp}{[1-(1-E^{\mathrm{sc}}+E_\perp)^2]^{1/2}} \times \left( 2 \int_0^{\arccos(1-E_\perp/2)} \arccos(2-E_\perp-\cos u)du - \left(\arccos\left(1-\frac{E_\perp}{2}\right)\right)^2 \right). \tag{A7}$$

In the next step, the function:

$$f(E^{\mathrm{sc}}, E_\perp) = 8 \arcsin(1-E^{\mathrm{sc}}+E_\perp) \tag{A8}$$

introduced to calculations gives:

$$N^{\mathrm{tot}}(E^{\mathrm{sc}}) = \int_0^{E^{\mathrm{sc}}} \frac{\partial f}{\partial E_\perp}(E^{\mathrm{sc}}, E_\perp) \cdot g^{\mathrm{sc}}(E_\perp) dE_\perp, \tag{A9}$$

where

$$g^{\mathrm{sc}}(E_\perp) = 2 \int_0^{\arccos(1-E_\perp/2)} \arccos(2-E_\perp-\cos u)du - \left(\arccos\left(1-\frac{E_\perp}{2}\right)\right)^2. \tag{A10}$$

The derivative function of $f$, *viz.*:

$$\frac{\partial f}{\partial E_\perp}(E^{\mathrm{sc}}, E_\perp) = \frac{8}{[1-(1-E^{\mathrm{sc}}+E_\perp)^2]^{1/2}}, \tag{A11}$$

is singular for $E_\perp = E^{\mathrm{sc}}$. In order to avoid this singularity in the differentiation process of (A9) with respect to $E^{\mathrm{sc}}$, we introduce the function:

$$f_\delta(E^{\mathrm{sc}}, E_\perp) = 8 \arcsin[(1-E^{\mathrm{sc}}+E_\perp)\delta], \tag{A12}$$

for some $0 < \delta < 1$ ($\delta \sim 1$), and obtain an expression for the approximate number of states:

$$N_\delta^{\mathrm{tot}}(E^{\mathrm{sc}}) = \int_0^{E^{\mathrm{sc}}} \frac{\partial f_\delta}{\partial E_\perp}(E^{\mathrm{sc}}, E_\perp) \cdot g^{\mathrm{sc}}(E_\perp) dE_\perp, \tag{A13}$$

dependent on $\delta$. Because of the relation:

$$\frac{\partial f_\delta}{\partial E_\perp}(E^{\rm sc},E_\perp)=\frac{8\delta}{[1-(1-E^{\rm sc}+E_\perp)^2\delta^2]^{1/2}}, \tag{A14}$$

the integrand of Equation (A13) is a well-defined function for all energies $E_\perp$ on the interval $0\le E_\perp\le E^{\rm sc}\le 2$. Now, the differentiation of (A13) with respect to $E^{\rm sc}$ gives:

$$\begin{aligned}\frac{dN_\delta^{\rm tot}(E^{\rm sc})}{dE^{\rm sc}}=&\int_0^{E^{\rm sc}}\frac{\partial^2 f_\delta}{\partial E^{\rm sc}\partial E_\perp}(E^{\rm sc},E_\perp)\cdot g^{\rm sc}(E_\perp)dE_\perp\\ &+\frac{\partial f_\delta}{\partial E_\perp}(E^{\rm sc},E_\perp)\cdot g^{\rm sc}(E_\perp)\Big|_{E_\perp=E^{\rm sc}}.\end{aligned} \tag{A15}$$

By the method of integration by parts, we arrive at:

$$\begin{aligned}\frac{dN_\delta^{\rm tot}(E^{\rm sc})}{dE^{\rm sc}}=&-\int_0^{E^{\rm sc}}\frac{\partial f_\delta}{\partial E^{\rm sc}}(E^{\rm sc},E_\perp)\cdot\frac{dg^{\rm sc}(E_\perp)}{dE_\perp}dE_\perp\\ &+\frac{\partial f_\delta}{\partial E^{\rm sc}}(E^{\rm sc},E_\perp)\cdot g^{\rm sc}(E_\perp)\Big|_{E_\perp=E^{\rm sc}}+\frac{\partial f_\delta}{\partial E_\perp}(E^{\rm sc},E_\perp)\cdot g^{\rm sc}(E_\perp)\Big|_{E_\perp=E^{\rm sc}}.\end{aligned} \tag{A16}$$

But in view of the definition of $f_\delta$ (see Equation (A12)):

$$\frac{\partial f_\delta}{\partial E^{\rm sc}}(E^{\rm sc},E_\perp)\cdot g^{\rm sc}(E_\perp)\Big|_{E_\perp=E^{\rm sc}}=-\frac{8\delta g^{\rm sc}(E^{\rm sc})}{(1-\delta^2)^{1/2}}, \tag{A17}$$

and

$$\frac{\partial f_\delta}{\partial E_\perp}(E^{\rm sc},E_\perp)\cdot g^{\rm sc}(E_\perp)\Big|_{E_\perp=E^{\rm sc}}=\frac{8\delta g^{\rm sc}(E^{\rm sc})}{(1-\delta^2)^{1/2}}. \tag{A18}$$

The results (A17) and (A18) simplify Equation (A16) into the formula:

$$\frac{dN_\delta^{\rm tot}(E^{\rm sc})}{dE^{\rm sc}}=-\int_0^{E^{\rm sc}}\frac{\partial f_\delta}{\partial E^{\rm sc}}(E^{\rm sc},E_\perp)\cdot\frac{dg^{\rm sc}(E_\perp)}{dE_\perp}dE_\perp. \tag{A19}$$

Here, the differentiation of Equation (A10) with respect to $E_\perp$ gives:

$$\frac{dg^{\rm sc}(E_\perp)}{dE_\perp}=2\int_0^{\arccos(1-E_\perp/2)}\frac{du}{[1-(2-E_\perp-\cos u)^2]^{1/2}}, \tag{A20}$$

which provides us with an approximate formula for the density of states (A19).

It can be demonstrated that the difference between Equation (A19) and the exact formula for the density of states, obtained by putting $\delta=1$ in Equation (A19), *viz.*:

$$N(E^{\rm sc})=\frac{dN^{\rm tot}(E^{\rm sc})}{dE^{\rm sc}}=-\int_0^{E^{\rm sc}}\frac{\partial f}{\partial E^{\rm sc}}(E^{\rm sc},E_\perp)\cdot\frac{dg^{\rm sc}(E_\perp)}{dE_\perp}dE_\perp, \tag{A21}$$

tends to zero while $\delta\longrightarrow 1$. Therefore, Equation (A19) applied in the limiting process of $\delta\longrightarrow 1$ can be used in the calculation of the $N(E^{\rm sc})$ data given in Table 1.

A similar integration calculation can be applied for $N(E^{\mathrm{bcc}})$, being the density of electron states in the bcc lattice (see Table 2). In this case, with the aid of Equations (17)–(19), we obtain:

$$N(E^{\mathrm{bcc}}) = \frac{dN^{\mathrm{tot}}(E^{\mathrm{bcc}})}{dE^{\mathrm{bcc}}} = 16 \int_0^{E^{\mathrm{bcc}}} \frac{dE_\perp}{[(1-E_\perp)^2 - (1-E^{\mathrm{bcc}})^2]^{1/2}} \times \int_0^{\arccos\sqrt{1-E_\perp}} \frac{du}{[\cos^2 u - (1-E_\perp)^2]^{1/2}}. \tag{A22}$$

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