

Analytic quadratic integration over the two-dimensional brillouion zone, G Wiesenekker, G te Velde and EJBaerends

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Contents

1	2D	3
1.1	$f = 1$ case	3
1.2	$f = r^2$ case	3
2	The limits on the u-integration of the goniometric equations	4
2.1	Ellipse	4
2.2	Hyperbola	4
2.3	Parabola	5
2.4	Straight line	5
2.5	Degenerate	5
3	Checking if a point is inside a triangle	6
4	What is next?	6

1 2D

$$E(k_x, k_y) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2) \quad (1)$$

The polar coordinate system

$$x = r \cos(\theta) \quad (2)$$

$$y = r \sin(\theta) \quad (3)$$

$$r = \sqrt{x^2 + y^2} \quad (4)$$

$$Jacobian = \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{vmatrix} = \begin{vmatrix} \cos(\theta) & -r \sin(\theta) \\ \sin(\theta) & r \cos(\theta) \end{vmatrix} = r$$

$$r^2 = (k_x^2 + k_y^2) = \frac{2mE}{\hbar^2} \quad (5)$$

$$\frac{\partial E}{\partial r} = \frac{\partial \frac{\hbar^2}{2m} r^2}{\partial r} = r \frac{\hbar^2}{m} \quad (6)$$

$$dr = dE \frac{m}{\hbar^2 r} \quad (7)$$

1.1 $f = 1$ case

and the main integral

$$D(E) = \int \delta(E - e(k)) dk \quad (8)$$

$$= \int_0^1 \int_0^{2\pi} r \delta(E - e(k)) d\theta dr \quad (9)$$

$$= \int 2\pi r \frac{m}{\hbar^2 r} \delta(E - e(k)) dE \quad (10)$$

$$= \int \frac{m2\pi}{\hbar^2} \delta(E - e(k)) dE \quad \text{where } \int f(E) \delta(E - e(k)) dE = f(e) \quad (11)$$

$$= \frac{2\pi m}{\hbar^2} \quad (12)$$

1.2 $f = r^2$ case

the main integral

$$D(E) = \int r^2 \delta(E - e(k)) dk \quad (13)$$

$$= \int_0^1 \int_0^{2\pi} r^3 \delta(E - e(k)) d\theta dr \quad (14)$$

$$= \int 2\pi r^3 \frac{m}{\hbar^2 r} \delta(E - e(k)) dE \quad (15)$$

$$= \int \frac{r^2 m 2\pi}{\hbar^2} \delta(E - e(k)) dE \quad \text{where } \int f(E) \delta(E - e(k)) dE = f(e) \quad (16)$$

$$= \frac{r^2 2\pi m}{\hbar^2} \quad (17)$$

$$= \left(\frac{2m}{\hbar^2} \right)^2 \pi E \quad (18)$$

2 The limits on the u-integration of the goniometric equations

the parameters specifying the intersection of the surface energy and with the sides of the triangle $n_{jx} + n_{jy} = c_j$ ref(41) to introduce the triangle sides we use the the stander formula for a line function $y = mx + b$, where m is the slope and b is the y-intercept the value of y in $x = 0$. and the point slope: $(y - y_1) = m(x - x_1)$ where (x_1, y_1) is a point in the given line.

$$y - y_1 = m(x - x_1) \quad (19)$$

$$y - y_1 = \frac{\partial y}{\partial x}(x - x_1) \quad (20)$$

$$\partial x(y - y_1) = \partial y(x - x_1) \quad (21)$$

$$\partial x y - \partial y x + \partial y x_1 - \partial x y_1 = 0 \quad (22)$$

$$n_{jx}x + n_{jy}y = c_j \quad \text{where } n_{jx} = -\partial y, n_{jy} = \partial x, c = \partial x y_1 - \partial y x_1 \quad (23)$$

2.1 Ellipse

the ellipse requires the solution of the goniometric equation ref (42)

$$n_{jx}\{(E - q_1)/q_4\}^{1/2}\cos(u) + n_{jy}\{(E - q_1)/q_6\}^{1/2}\sin(u) = c_j \quad \text{where } (j = 1, 2, 3) \quad (24)$$

$$b\cos(u) + a\sin(u) = c_j \quad (25)$$

$$t = \tan\left(\frac{u}{2}\right) \quad (26)$$

$$\sin(u) = 2\sin\left(\frac{u}{2}\right)\cos\left(\frac{u}{2}\right) = 2\frac{\sin(\frac{u}{2})}{\cos(\frac{u}{2})}\cos^2\left(\frac{u}{2}\right) = \frac{2\tan(\frac{u}{2})}{\sec^2(\frac{u}{2})} = \frac{2t}{1+t^2} \quad (27)$$

$$\cos(u) = \cos^2\left(\frac{u}{2}\right) - \sin^2\left(\frac{u}{2}\right) = \left[1 - \frac{\sin^2(\frac{u}{2})}{\cos^2(\frac{u}{2})}\right]\cos^2\left(\frac{u}{2}\right) = \frac{1 - \tan^2(\frac{u}{2})}{\sec^2(\frac{u}{2})} = \frac{1 - t^2}{1 + t^2} \quad (28)$$

$$(29)$$

$$a_j\left(\frac{2t}{1+t^2}\right) + b_j\left(\frac{1-t^2}{1+t^2}\right) = c_j \quad 25 \quad (30)$$

$$a_j 2t + b_j(1 - t^2) = c_j(1 + t^2) \quad (31)$$

$$(c_j + b_j)t^2 - a_j 2t + (c_j - b_j) = 0 \quad (32)$$

solving the Quadratic equations 32 gives us

$$t_j = \frac{2a_j \pm \sqrt{4a_j^2 - 4(c_j - b_j)(b_j + c_j)}}{2(b_j + c_j)} \quad (33)$$

$$u_j = 2\tan^{-1}(t_j) \quad \text{for } (j = 1, 2, 3) \quad (34)$$

which give two solutions for each j:

$$u = u_1, u_2, u_3, u_4, u_5, u_6 \quad (35)$$

2.2 Hyperbola

The hyperbola form need a solution for the quadratic equation: ref (43)

$$n_{jx}u^2 - c_j u + n_{jy}\{(E - q_1)/q_5\} = 0 \quad \text{where } (j = 1, 2, 3) \quad (36)$$

$$a'_j u^2 + b'_j u + c'_j = 0 \quad (37)$$

We can find the solution for u by using the quadratic formula:

$$u_j = \frac{-b'_j \pm \sqrt{b'^2_j - 4a'_j c'_j}}{2a'_j} \quad (38)$$

which give 2 solutions for each j :

$$u = u_1, u_2, u_3, u_4, u_5, u_6 \quad (39)$$

2.3 Parabola

The Parabola form need a solution for the quadratic equation: ref (44)

$$-n_{jy}(q_4/q_3)u^2 + n_{jx}u + n_{jy}\{(E - q_1)/q_3\} - c_j = 0 \quad \text{where } (j = 1, 2, 3) \quad (40)$$

$$a'_j u^2 + b'_j u + c'_j = 0 \quad (41)$$

We can find the solution for u by using the quadratic formula:

$$u_j = \frac{-b'_j \pm \sqrt{b'^2_j - 4a'_j c'_j}}{2a'_j} \quad (42)$$

which give two solutions for each j :

$$u = u_1, u_2, u_3, u_4, u_5, u_6 \quad (43)$$

2.4 Straight line

The straight line form need a solution for the equation: ref (45)

$$n_{jy}u + n_{jx}\{(E - q_1)/q_2\} - c_j = 0 \quad \text{where } (j = 1, 2, 3) \quad (44)$$

$$u = \frac{c_j - \{(E - q_1)/q_2\}}{n_{jy}} \quad (45)$$

which give one solutions for each j :

$$u = u_1, u_2, u_3 \quad (46)$$

2.5 Degenerate

The degenerate form $E_q(x, y) = q_1 + q_4 x^2$ need a solution for the equation of the two parallel lines : ref (38,39,40)

$$x = \pm \{(e - q_1)/q_4\}^{1/2} \quad (47)$$

with the parametrsation:

$$x = \pm (e - q_1)/\{q_4(e - q_1)\}^{1/2} \quad y = u \quad (48)$$

The degenerate form need a solution of the equation ref (41)

$$n_{jx}x + n_{jy}y = c_j \quad (49)$$

$$n_{jx}(e - q_1)/\{q_4(e - q_1)\}^{1/2} + n_{jy}u = c_j \quad (50)$$

$$u = \frac{c_j - n_{jx}(e - q_1)/\{q_4(e - q_1)\}^{1/2}}{n_{jy}} \quad (51)$$

The Jacobian is:

$$\left[\frac{\partial(x, y)}{\partial(e, u)} \right] = 1/2 \{q_4(e - q_1)\}^{1/2} \quad (52)$$

The integral become

$$V_1 = \int_{e, u} \delta(E - e) 1/2 \{q_4(e - q_1)\}^{1/2} de du = 1/2 \{q_4(e - q_1)\}^{1/2} [u] \quad (53)$$

$$V_2 = \pm 1/2 \{q_4(e - q_1)\}^{1/2} (e - q_1) / \{q_4(e - q_1)\}^{1/2} [u] \quad (54)$$

$$V_3 = \pm 1/2 \{q_4(e - q_1)\}^{1/2} [\frac{1}{2} u^2] \quad (55)$$

$$V_4 = \pm 1/2 \{q_4(e - q_1)\}^{1/2} (e - q_1)^2 / \{q_4(e - q_1)\} [u] \quad (56)$$

$$V_5 = \pm 1/2 \{q_4(e - q_1)\}^{1/2} (e - q_1) / \{q_4(e - q_1)\}^{1/2} [\frac{1}{2} u^2] \quad (57)$$

$$V_6 = \pm 1/2 \{q_4(e - q_1)\}^{1/2} [\frac{1}{3} u^3] \quad (58)$$

$$(59)$$

which give one solutions for each j:

$$u = u_1, u_2, u_3 \quad (60)$$

3 Checking if a point is inside a triangle

This simple check can tell us if the curve lies inside the triangle. The test give an existed point in the triangle area only if :

$$p(x, y) = c_0 + (c_1 - c_0) * s + (c_2 - c_0) * t \quad (61)$$

c_0, c_1, c_2 is the three corners of the triangle

the point p is inside the triangle if and only if $0 < S < 1$, $0 < t < 1$ and $s + t < 1$.

4 What is next?

with this integration method we can get good but slow result but this will be enough to make a machine learning program which can calc much faster and better result with much lower k points. but first we need to a huge data set "learning set" .