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

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Contents

1 2D

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

The polar coordinate system

$$x = rcos(\theta) \tag{2}$$
$$y = rsin(\theta) \tag{3}$$
$$r = \sqrt{x^2+y^2} \tag{4}$$

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

$$r^2 = (k_x^2+k_y^2) = \frac{2mE}{\hbar^2} \tag{5}$$
$$\frac{\partial E}{\partial r} = \frac{\partial \frac{\hbar^2}{2m} r^2}{\partial r} = r\frac{\hbar^2}{m} \tag{6}$$
$$dr = dE\frac{m}{\hbar^2 r} \tag{7}$$

1.1 $f = 1$ case

and the main integral

$$D(E) = \int \delta(E-e(k))dk \tag{8}$$
$$= \int_0^1 \int_0^{2\pi} r\delta(E-e(k))d\theta dr \tag{9}$$
$$= \int 2\pi r \frac{m}{\hbar^2 r}\delta(E-e(k))dE \tag{10}$$
$$= \int \frac{m2\pi}{\hbar^2}\delta(E-e(k))dE \qquad \textbf{where} \int f(E)\delta(E-e(k))dE = f(e) \tag{11}$$
$$= \frac{2\pi m}{\hbar^2} \tag{12}$$

1.2 $f = r^2$ case

the main integral

$$D(E) = \int r^2\delta(E-e(k))dk \tag{13}$$
$$= \int_0^1 \int_0^{2\pi} r^3\delta(E-e(k))d\theta dr \tag{14}$$
$$= \int 2\pi r^3 \frac{m}{\hbar^2 r}\delta(E-e(k))dE \tag{15}$$
$$= \int \frac{r^2 m2\pi}{\hbar^2}\delta(E-e(k))dE \qquad \textbf{where} \int f(E)\delta(E-e(k))dE = f(e) \tag{16}$$
$$= \frac{r^2 2\pi m}{\hbar^2} \tag{17}$$
$$= \left(\frac{2m}{\hbar^2}\right)^2 \pi E \qquad 5 \tag{18}$$

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.

$$y - y_1 = m(x - x_1) \tag{19}$$

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

$$\partial x(y - y_1) = \partial y(x - x_1) \tag{21}$$

$$\partial xy - \partial yx + \partial yx_1 - \partial xy_1 = 0 \tag{22}$$

$$n_{jx}x + n_{jy}y = c_j \qquad \text{where } n_{jx} = -\partial y, n_{jy} = \partial x, c = \partial xy_1 - \partial yx_1 \tag{23}$$

2.1 Ellipse

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

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

$$bcos(u) + asin(u) = c_j \tag{25}$$

$$t = tan(\frac{u}{2}) \tag{26}$$

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

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

$$\tag{29}$$

$$a_j(\frac{2t}{1+t^2}) + b_j(\frac{1-t^2}{1+t^2}) = c_j \qquad 25 \tag{30}$$

$$a_j 2t + b_j(1 - t^2) = c_j(1 + t^2) \tag{31}$$

$$(c_j + b_j)t^2 - a_j 2t + (c_j - b_j) = 0 \tag{32}$$

solving the Quadratic equations 32 gives us

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

$$u_j = 2tan^{-1}(t_j) \qquad \textbf{for } (j = 1,2,3) \tag{34}$$

which give two solutions for each j:

$$u = u_1, u_2, u_3, u_4, u_5, u_6 \tag{35}$$

2.2 Hyperbola

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

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

$$a'_j u^2 + b'_j u + c'_j = 0 \tag{37}$$

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

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

which give 2 solutions for each j:

$$u = u_1, u_2, u_3, u_4, u_5, u_6 \tag{39}$$

2.3 Parabola

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

$$-n_{jy}(q_4/q_3)u^2 + n_{jx}u + n_{jy}\{(E-q_1)/q3\} - c_j = 0 \qquad \text{where } (j = 1,2,3) \tag{40}$$

$$a'_j u^2 + b'_j u + c'_j = 0 \tag{41}$$

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

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

which give two solutions for each j:

$$u = u_1, u_2, u_3, u_4, u_5, u_6 \tag{43}$$

2.4 Straight line

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

$$n_{jy}u + n_{jx}\{(E-q_1)/q2\} - c_j = 0 \qquad \text{where } (j = 1,2,3) \tag{44}$$

$$u = \frac{c_j - \{(E-q_1)/q2\}}{n_{jy}} \tag{45}$$

which give one solutions for each j:

$$u = u_1, u_2, u_3 \tag{46}$$

2.5 Degenerate

The degenerate form $E_q(x, y) = q_1 + q_4x^2$ need a solution for the equation of the two parallel lines : ref (38,39,40)

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

with the parametrsation:

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

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

$$n_{jx}x + n_{jy}y = c_j \tag{49}$$

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

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

The Jacobian is:

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

The integral become

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

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

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

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

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

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

$$\tag{59}$$

which give one solutions for each j:

$$u = u_1, u_2, u_3 \tag{60}$$

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 :

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

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 3D

need to include the stander triangel in 2D and the weight consept i have them on paper, and need to adde the stander tettrahedral

4.1 Standard tetrahedron

Any tetrahedron with corners (c_1, c_2, c_3, c_4) can be transformed to the standard tetrahedron with corners (0,0,0), (1,0,0), (0,1,0) and (0,0,1) by the affine transformation. $f_q(x,y,z) = p_1 + p_2x + p_3y + p_4z + P_5x^2 + p_6xy + p_7xz + p8y^2 + p6yz + p_10z^2$

$$F = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0.5 & 0 & 0 & 0.25 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0.5 & 0 & 0 & 0 & 0 & 0.25 & 0 & 0 \\ 1 & 0 & 0 & 0.5 & 0 & 0 & 0 & 0 & 0 & 0.25 \\ 1 & 0.5 & 0.5 & 0 & 0.25 & 0.25 & 0 & 0.25 & 0 & 0 \\ 1 & 0 & 0.5 & 0.5 & 0 & 0 & 0 & 0.25 & 0.25 & 0.25 \\ 1 & 0.5 & 0 & 0.5 & 0.25 & 0 & 0.25 & 0 & 0 & 0.25 \end{bmatrix}$$

$$FI = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -3 & -1 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ -3 & 0 & -1 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ -3 & 0 & 0 & -1 & 0 & 0 & 4 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & -4 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & -4 & -4 & 0 & 4 & 0 & 0 \\ 4 & 0 & 0 & 0 & -4 & 0 & -4 & 0 & 0 & 4 \\ 2 & 0 & 2 & 0 & 0 & -4 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 & -4 & -4 & 0 & 4 & 0 \\ 2 & 0 & 0 & 2 & 0 & 0 & -4 & 0 & 0 & 0 \end{bmatrix}$$

4.2 3D-z

we need to find the coordinates for each triangle for each Z-point we chose in our numerical integration. if we chose z = 0 , we get our tetrahdral base. (0,0), (1,0) , (0,1). parameterizing to z. z form 0 to 1: $(0,0),(1-z,0),(0,1-z),(\frac{1-z}{2},0),(0,\frac{1-z}{2}),(\frac{1-z}{2},\frac{1-z}{2})$

5 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" .