1 Integral with Fermi-sphere constraints

a. Intersection of two spheres

Solution: First I'm going to argue that

$$\Theta(k_F - |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|),$$

is a sphere centered on $-\boldsymbol{q}/2$ with radius k_F. Let's analyze this, the Heaviside function is going to be zero whenever

$$k_F - |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}| < 0,$$
$$k_F < |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|.$$

In other words, it will be 1 if the next condition is fulfilled

$$k_F > |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|.$$

So, the value will be non-zero just when $|\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|$ is less than k_F. And by definition this is a ball. Where is the center of this ball? We are tempted to say that in $\boldsymbol{q}/2$, since $\boldsymbol{P}$ is the variable changing, and we are measuring the distance from $\boldsymbol{P}$ to $\boldsymbol{q}/2$. But let's remember that the distance between two vectors is $|\boldsymbol{a} - \boldsymbol{b}|$, not $|\boldsymbol{a} + \boldsymbol{b}|$. So $|\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|$ is the distance between $\boldsymbol{P}$ and $-\boldsymbol{q}/2$. Hence the center of the sphere is naturally at $-\boldsymbol{q}/2$.

The same arguments can be used to show that

$$\Theta(k_F - |\boldsymbol{P} - \frac{1}{2}\boldsymbol{q}|),$$

is a sphere of radius k_F centered at $\boldsymbol{q}/2$. As a consequence of this we can easily notice that the integral

$$\int d\boldsymbol{P}\Theta(k_F - |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|)\Theta(k_F - |\boldsymbol{P} - \frac{1}{2}\boldsymbol{q}|), \tag{1}$$

is the volume of the intersection of the two spheres. The volume is then (taken from `http://mathworld.wolfram.com/Sphere-SphereIntersection.html`)

$$\begin{aligned}
\int d\boldsymbol{P}\Theta(k_F - |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|)\Theta(k_F - |\boldsymbol{P} - \frac{1}{2}\boldsymbol{q}|) &= \frac{\pi}{12}(4k_F + q)(2k_F - q)^2, \\
&= \frac{\pi}{12}(16k_F^3 - 12k_F^2 q + q^3), \\
&= \frac{16\pi}{12}(k_F^3 - \frac{12}{16}k_F^2 q + \frac{q^3}{16}), \\
&= \frac{16\pi}{12}k_F^3(1 - \frac{12}{16k_F}q + \frac{q^3}{16k_F^3}), \\
&= \frac{16\pi}{12}k_F^3(1 - \frac{3x}{2} + \frac{x^3}{2}),
\end{aligned}$$

And this is almost true, except that this is true only when they intersect. The spheres will intersect when the distance between the two centers is less that $2k_F$, in equations this is

$$q < 2k_F,$$

or equivalently

$$\frac{q}{2k_F} < 1. \tag{2}$$

Then, we need to multiply the volume by a function that is zero when $\frac{q}{2k_F} > 1$ and 1 otherwise (remember that q and k_F are positive numbers). Fortunately we know such function, it will be $\Theta(1-x)$, with $x = q/2k_F$. Finally we can multiply for that function and get

$$\int d\boldsymbol{P}\Theta(k_F - |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|)\Theta(k_F - |\boldsymbol{P} - \frac{1}{2}\boldsymbol{q}|) = \frac{4\pi}{3}k_F^3(1 - \frac{3x}{2} + \frac{x^3}{2})\Theta(1-x). \quad \blacksquare \tag{3}$$

Finally we can move to the last integral, but first let's do this, if $x = q/2k_F$ then

$$q = 2xk_F, \tag{4}$$

and also

$$\begin{aligned} \frac{dx}{dq} &= \frac{1}{2k_F}, \\ \Rightarrow dq &= 2k_F dx. \end{aligned} \tag{5}$$

Now, the integral we need to calculate is

$$\frac{1}{(2\pi)^6}\int d\boldsymbol{q}\frac{4\pi}{q^2}\int d\boldsymbol{P}\Theta(k_F - |\boldsymbol{P} + \frac{1}{2}\boldsymbol{q}|)\Theta(k_F - |\boldsymbol{P} - \frac{1}{2}\boldsymbol{q}|).$$

using eqs. 4-5, and integrating in spherical coordinates we have

$$\begin{aligned}
&\frac{1}{(2\pi)^6}\int d\boldsymbol{q}\frac{4\pi}{q^2}\left(\frac{4\pi}{3}k_F^3(1 - \frac{3x}{2} + \frac{x^3}{2})\Theta(1-x)\right), \\
=&\frac{(4\pi)^2}{3(2\pi)^6}\int d\boldsymbol{q}\frac{1}{q^2}\left(k_F^3(1 - \frac{3x}{4} + \frac{x^3}{2})\Theta(1-x)\right), \\
=&\frac{(4\pi)^2}{3(2\pi)^6}\int d\theta\sin(\phi)d\phi dq q^2\frac{1}{q^2}\left(k_F^3(1 - \frac{3x}{2} + \frac{x^3}{2})\Theta(1-x)\right), \\
=&\frac{(4\pi)^2}{3(2\pi)^6}\int d\theta\sin(\phi)d\phi 2k_F dx\left(k_F^3(1 - \frac{3x}{4} + \frac{x^3}{2})\Theta(1-x)\right), \\
=&\frac{(4\pi)^2}{(2\pi)^6}\frac{2k_F}{3}\overbrace{\int_0^{2\pi}d\theta}^{2\pi}\overbrace{\int_0^{\pi}\sin(\phi)d\phi}^{2}\int dx\left(k_F^3(1 - \frac{3x}{2} + \frac{x^3}{2})\Theta(1-x)\right), \\
=&\frac{(4\pi)^3}{(2\pi)^6}\frac{2k_F^4}{3}\int dx\left((1 - \frac{3x}{2} + \frac{x^3}{2})\Theta(1-x)\right), \\
=&\frac{(4\pi)^3}{(2\pi)^6}\frac{2k_F^4}{3}\int_0^1 dx\left((1 - \frac{3x}{2} + \frac{x^3}{2})\right), \\
=&\frac{(4\pi)^3}{(2\pi)^6}\frac{2k_F^4}{3}\left((x - \frac{3x^2}{4} + \frac{x^4}{8})\right)\Bigg|_0^1, \\
=&\frac{(4\pi)^3}{(2\pi)^6}\frac{2k_F^4}{3}\left((1 - \frac{3}{4} + \frac{1}{8})\right) = \frac{(4\pi)^3}{(2\pi)^6}\frac{2k_F^4}{3}\frac{3}{8} = \frac{4^3\pi^3}{4^3\pi^6}\frac{2k_F^4}{8} = \frac{k_F^4}{4\pi^3}.
\end{aligned}$$

2 Density of states

a. DOS in 1D

Solution: Let's start by setting the integral we need to solve for the three cases

$$\rho(\epsilon) = 2\int \frac{1}{(2\pi)^N} d\boldsymbol{k}\delta(\epsilon(k) - \varepsilon), \tag{6}$$

where N is the dimensionality of the space.

This been said, let's solve the problem for 1 dimension first.

$$\begin{aligned} \rho_{1D}(\epsilon) &= 2\int \frac{1}{2\pi} dk\delta(\epsilon(k) - \varepsilon), \\ &= \frac{1}{\pi}\int dk\delta(\epsilon(k) - \varepsilon), \end{aligned} \tag{7}$$

Let's put this on hold a second to propose a variable change from k to ϵ, we know that

$$\epsilon = \frac{k^2}{2}, \tag{8}$$

therefore

$$\frac{d\epsilon}{dk} = 2k, \Rightarrow dk = \frac{d\epsilon}{2k}, \tag{9}$$

plugging this on eq. 7 we will have

$$\begin{aligned} \rho_{1D}(\epsilon) &= \frac{1}{\pi}\int \frac{d\epsilon}{2k(\epsilon)}\delta(\epsilon - \varepsilon), \\ &= \frac{1}{2\pi k(\varepsilon)}, \\ &= \frac{1}{2\pi\sqrt{2\varepsilon}}, \quad \text{using eq. 8} \end{aligned} \tag{10}$$

b. DOS in 2D

Solution: Again using eq. 6 the problem we need to solve for 2D is

$$\rho(\epsilon) = 2\int \frac{1}{(2\pi)^2} d\boldsymbol{k}\delta(\epsilon(k) - \varepsilon), \tag{11}$$

Now $\boldsymbol{dk}$ is a vector quantity, let's use spherical coordinates for this and write $d\boldsymbol{k} = kdkd\theta$

$$\begin{aligned} \rho(\epsilon) &= \frac{2}{(2\pi)^2} \int \delta(\epsilon(k) - \varepsilon) kdkd\theta, \\ &= \frac{2}{(2\pi)^2} \int \delta(\epsilon(k) - \varepsilon) kdk \int_0^{2\pi} d\theta, \\ &= \frac{2(2\pi)}{(2\pi)^2} \int \delta(\epsilon(k) - \varepsilon) kdk, \\ &= \frac{1}{\pi} \int \delta(\epsilon(k) - \varepsilon) kdk, \\ &= \frac{1}{\pi} \int \delta(\epsilon(k) - \varepsilon) k\frac{d\epsilon}{2k}, \quad \text{using eq 9}, \\ &= \frac{1}{2\pi} \int \delta(\epsilon - \varepsilon) d\epsilon, \\ &= \frac{1}{2\pi}. \end{aligned} \tag{12}$$

c. DOS in 3D

Solution: Finally we are ready to face the boss of this level. The density of states in 3D. Let's set the integral we need to solve

$$\rho(\epsilon) = 2 \int \frac{1}{(2\pi)^3} d\boldsymbol{k} \delta(\epsilon(k) - \varepsilon). \tag{13}$$

As in the previous exercise we are going to use spherical coordinates but now in $\mathbb{R}^3$

$$\begin{aligned} \rho(\epsilon) &= \frac{2}{(2\pi)^3} \int \delta(\epsilon(k) - \varepsilon) k^2 \sin\theta dkd\phi d\phi, \\ &= \frac{2}{(2\pi)^3} \int \delta(\epsilon(k) - \varepsilon) k^2 dk \cancelto{2\pi}{\int_0^{2\pi} d\theta} \cancelto{2}{\int_0^{\pi} \sin\phi d\phi}, \\ &= \frac{4(2\pi)}{(2\pi)^3} \int \delta(\epsilon(k) - \varepsilon) k^2 dk, \\ &= \frac{4}{(2\pi)^2} \int \delta(\epsilon - \varepsilon) k^2(\epsilon) \frac{d\epsilon}{2k}, \quad \text{using eq. 9}, \\ &= \frac{2}{(2\pi)^2} \int \delta(\epsilon - \varepsilon) k(\epsilon) d\epsilon, \\ &= \frac{2}{(2\pi)^2} k(\varepsilon) = \frac{2}{(2\pi)^2} \sqrt{2\epsilon}. \end{aligned} \tag{14}$$

3 Reciprocal lattice

a. $\exp(i\vec{G} \cdot \vec{T}) = 1$

Solution: Let's begin with the definition of the reciprocal basis vectors b_i

$$\boldsymbol{b}_i = 2\pi \frac{\boldsymbol{a}_j \times \boldsymbol{a}_k}{\boldsymbol{a}_i \cdot (\boldsymbol{a}_j \times \boldsymbol{a}_k)} \epsilon_{ijk}, \tag{15}$$

where ϵ_{ijk} is the Levy-Civitta symbol, and $\boldsymbol{a}_i$ are the direct basis vectors. Let's move forward and define this two vectors,

$$\boldsymbol{T} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3 \qquad n_i \in \mathbb{Z}, \tag{16}$$

$$\boldsymbol{G} = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2 + m_3\boldsymbol{b}_3 \qquad m_i \in \mathbb{Z}. \tag{17}$$

From eq. 15 it is easy to notice that $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$, we will use this fact on the next step. Now, let's compute the following dot product

$$\begin{aligned}
\boldsymbol{G} \cdot \boldsymbol{T} &= (n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3) \cdot (m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2 + m_3\boldsymbol{b}_3), \\
&= n_1\boldsymbol{a}_1 \cdot (m_1\boldsymbol{b}_1 + \cancelto{0}{m_2\boldsymbol{b}_2} + \cancelto{0}{m_3\boldsymbol{b}_3}) \\
&+ n_2\boldsymbol{a}_2 \cdot (\cancelto{0}{m_1\boldsymbol{b}_1} + m_2\boldsymbol{b}_2 + \cancelto{0}{m_3\boldsymbol{b}_3}) \\
&+ n_3\boldsymbol{a}_3 \cdot (\cancelto{0}{m_1\boldsymbol{b}_1} + \cancelto{0}{m_2\boldsymbol{b}_2} + m_3\boldsymbol{b}_3), \\
&= n_1 m_1 \cancelto{2\pi}{\boldsymbol{a}_1 \cdot \boldsymbol{b}_1} + n_2 m_2 \cancelto{2\pi}{\boldsymbol{a}_2 \cdot \boldsymbol{b}_2} + n_3 m_3 \cancelto{2\pi}{\boldsymbol{a}_3 \cdot \boldsymbol{b}_3}, \\
&= 2\pi(n_1 m_1 + n_2 m_2 + n_3 m_3), \\
&= 2\pi\gamma, \qquad \gamma \in \mathbb{Z}.
\end{aligned} \tag{18}$$

Where in the last step we used the fact that $n_i, m_j \in \mathbb{Z}$. Now it's trivial to prove what we wanted to prove.

$$\exp(i\boldsymbol{G} \cdot \boldsymbol{T}) = \exp(2\pi i \gamma) = 1. \quad \blacksquare \tag{19}$$

b. Reciprocal of a cubic lattice

Solution: For this exercise I will use the following vector identity

$$(\boldsymbol{a} \times \boldsymbol{b}) \cdot (\boldsymbol{c} \times \boldsymbol{d}) = (\boldsymbol{a} \cdot \boldsymbol{c})(\boldsymbol{b} \cdot \boldsymbol{d}) - (\boldsymbol{a} \cdot \boldsymbol{d})(\boldsymbol{b} \cdot \boldsymbol{c}). \tag{20}$$

Now from equation 15 I will compute $\boldsymbol{b}_i \cdot \boldsymbol{b}_\alpha$, for the case when $i \neq \alpha$.

$$\begin{aligned}
\boldsymbol{b}_i \cdot \boldsymbol{b}_\alpha &= \left(2\pi \frac{\boldsymbol{a}_j \times \boldsymbol{a}_k}{\boldsymbol{a}_i \cdot (\boldsymbol{a}_j \times \boldsymbol{a}_k)} \epsilon_{ijk}\right) \cdot \left(2\pi \frac{\boldsymbol{a}_\beta \times \boldsymbol{a}_\gamma}{\boldsymbol{a}_\alpha \cdot (\boldsymbol{a}_\beta \times \boldsymbol{a}_\gamma)} \epsilon_{\alpha\beta\gamma}\right) \\
&= C(\boldsymbol{a}_j \times \boldsymbol{a}_k) \cdot (\boldsymbol{a}_\beta \times \boldsymbol{a}_\gamma), \\
&= C((\boldsymbol{a}_j \cdot \boldsymbol{a}_\beta)(\boldsymbol{a}_k \cdot \boldsymbol{a}_\gamma) - (\boldsymbol{a}_j \cdot \boldsymbol{a}_\gamma)(\boldsymbol{a}_k \cdot \boldsymbol{a}_\beta)).
\end{aligned} \tag{21}$$

At this point we need to be really smart (maybe normal-smart), first to notice that C absorbed all the non-vector quantities, because for reasons that will become clear soon, we don't care about them. And second, to know that the $\boldsymbol{a}_i$ basis has tree vectors but on eq. 21 we have 4 vectors. So we must have one vector repeated, once with italic index and once with greek index (by definition it can't have both latin or greek indexes), we can have two repeated vectors because this would lead to $\boldsymbol{b}_\alpha = \boldsymbol{b}_i$. Therefore one of the latin indexed vectors is no repeated on the greek indexed part. Using this and the fact that $\boldsymbol{a}_i \cdot \boldsymbol{a}_j = a^2\delta_{ij}$ we can unravel the mystery. Let's suppose without loss of generality that j is the index such that $j \neq \beta, \gamma$ and see how this influences our calculations

$$\begin{aligned}
\boldsymbol{b}_i \cdot \boldsymbol{b}_\alpha &= C((\cancelto{0}{\boldsymbol{a}_j \cdot \boldsymbol{a}_\beta})(\boldsymbol{a}_k \cdot \boldsymbol{a}_\gamma) - (\cancelto{0}{\boldsymbol{a}_j \cdot \boldsymbol{a}_\gamma})(\boldsymbol{a}_k \cdot \boldsymbol{a}_\beta)), \\
&= 0.
\end{aligned} \tag{22}$$

Therefore $\boldsymbol{b}_i \cdot \boldsymbol{b}_\alpha = 0$ if $i \neq \alpha$, and we can conclude that the reciprocal lattice is also cubic. ■

c. Brillouin zone

Solution: The Brillouin zone can be found as the Wigner-Seitz cell of every lattice point. To find it we can trace lines to first neighbors and the medians to those lines. The area enclosed inside the medians will be the Brillouin zone. The lattice will look like this

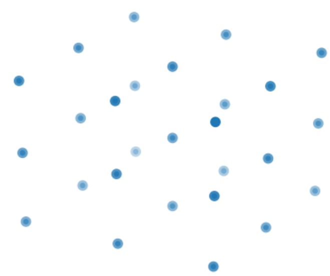

Figure 1: Reciprocal lattice in k space

The Brillouin zone will be then as shown in the following figures

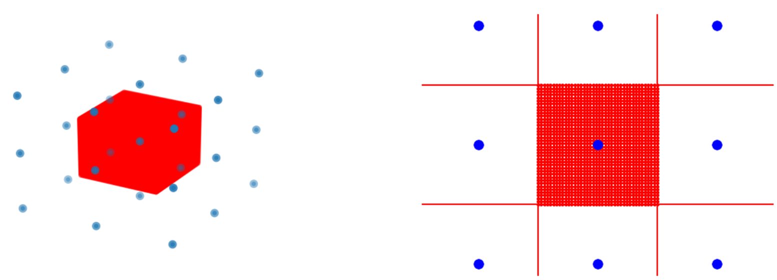

Figure 2: Brillouin zone on 3D (left side) and contour plot for $z = 0$ (right).

Finally, how would I find it numerically.
Honestly I would Google algorithms to find Voronoi-Diagrams because there must be pretty inteligent algorithms to do that. But if that's not a possibility I would to the following

1. Generate a finer mesh.
2. Travel along the points of this mesh.
3. For each point detect what lattice points are near.
4. Measure the distance to all of them.
5. Assign that mesh point to the closest lattice point.