**Department of physics, NTNU**
**TFY4340 Mesoscopic Physics**
**Spring 2010**

# Solution to Exercise 1

*Question 1*

We use the given vector identity, with $\boldsymbol{A} = \boldsymbol{a}_2$, $\boldsymbol{B} = \boldsymbol{a}_3$, and $\boldsymbol{C} = \boldsymbol{a}_3 \times \boldsymbol{a}_1$:

$$\begin{aligned}
V\tilde{V} &= V\,|\,(\boldsymbol{b}_1 \times \boldsymbol{b}_2)\cdot \boldsymbol{b}_3| \\
&= V\left(\frac{2\pi}{V}\right)^3 |\,((\boldsymbol{a}_2 \times \boldsymbol{a}_3) \times (\boldsymbol{a}_3 \times \boldsymbol{a}_1)) \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)\,| \\
&= V\left(\frac{2\pi}{V}\right)^3 |\,((\boldsymbol{a}_2 \cdot (\boldsymbol{a}_3 \times \boldsymbol{a}_1))\,\boldsymbol{a}_3 - (\boldsymbol{a}_3 \cdot (\boldsymbol{a}_3 \times \boldsymbol{a}_1))\,\boldsymbol{a}_2) \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)\,| \\
&= V\left(\frac{2\pi}{V}\right)^3 |V\boldsymbol{a}_3 \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)\,| \\
&= V\left(\frac{2\pi}{V}\right)^3 |V \cdot V| \\
&= (2\pi)^3
\end{aligned}$$

Here, we used the fact that $\boldsymbol{a}_3 \cdot (\boldsymbol{a}_3 \times \boldsymbol{a}_1) = 0$.

*Question 2*

We have two primitive vectors in direct space, $\boldsymbol{a}_i = (a_{ix}, a_{iy})$ $(i = 1, 2)$, and two in reciprocal space, $\boldsymbol{b}_i = (b_{ix}, b_{iy})$ $(i = 1, 2)$, and four equations relating them, $\boldsymbol{b}_i \cdot \boldsymbol{a}_j = 2\pi\delta_{ij}$ $(i, j = 1, 2)$. These four equations are exactly what we need in order to determine the four unknowns $b_{ix}, b_{iy}$ $(i = 1, 2)$. A little algebra yields

$$\begin{aligned}
b_{1x} &= \frac{2\pi a_{2y}}{a_{1x}a_{2y} - a_{1y}a_{2x}} \\
b_{1y} &= \frac{2\pi a_{2x}}{a_{1y}a_{2x} - a_{1x}a_{2y}} \\
b_{2x} &= \frac{2\pi a_{1y}}{a_{2x}a_{1y} - a_{2y}a_{1x}} \\
b_{2y} &= \frac{2\pi a_{1x}}{a_{2y}a_{1x} - a_{2x}a_{1y}}
\end{aligned}$$

With a regular hexagonal lattice, with nearest neighbour distance $a$, we have

$$\begin{aligned}
\boldsymbol{a}_1 &= a\hat{x} + a\cos(\pi/3)\hat{x} - a\sin(\pi/3)\hat{y} = \frac{3a}{2}\hat{x} - \frac{\sqrt{3}a}{2}\hat{y} \\
\boldsymbol{a}_2 &= a\hat{x} + a\cos(\pi/3)\hat{x} + a\sin(\pi/3)\hat{y} = \frac{3a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}
\end{aligned}$$

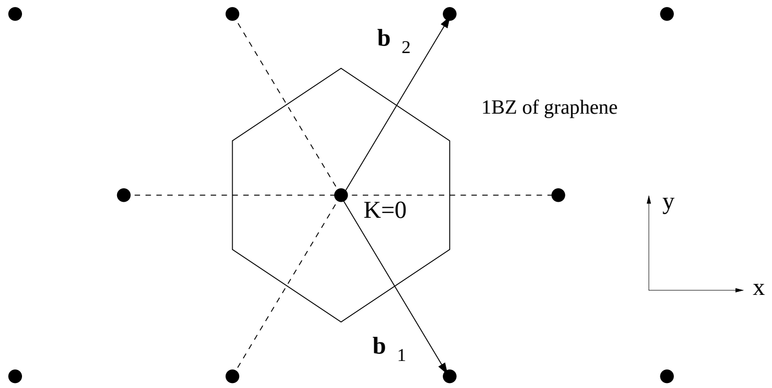
which yields

$$
\begin{aligned}
b_{1x} &= \frac{2\pi}{3a} \\
b_{1y} &= -\frac{2\pi}{\sqrt{3}a} \\
b_{2x} &= \frac{2\pi}{3a} \\
b_{2y} &= \frac{2\pi}{\sqrt{3}a}
\end{aligned}
$$

In other words, the reciprocal lattice is triangular, with primitive lattice vectors

$$
\begin{aligned}
\boldsymbol{b}_1 &= \frac{2\pi}{3a}\left(\hat{x} - \sqrt{3}\hat{y}\right) \\
\boldsymbol{b}_2 &= \frac{2\pi}{3a}\left(\hat{x} + \sqrt{3}\hat{y}\right)
\end{aligned}
$$

with magnitude $|\boldsymbol{b}_1| = |\boldsymbol{b}_2| = b = 4\pi/3a$. The first Brillouin zone is the area of $k$–space around the lattice point $\boldsymbol{K} = 0$ that is closer to the origin than to any other point of the reciprocal lattice, i.e., the so–called Wigner–Seitz cell. With a triangular reciprocal lattice, the 1BZ becomes hexagonal:




The area of the primitive cell in direct space is

$$
A = |\boldsymbol{a}_1 \times \boldsymbol{a}_2| = |a_{1x}a_{2y} - a_{1y}a_{2x}| = \frac{3\sqrt{3}a^2}{2},
$$

and the corresponding area in reciprocal space is

$$
\tilde{A} = |\boldsymbol{b}_1 \times \boldsymbol{b}_2| = |b_{1x}b_{2y} - b_{1y}b_{2x}| = \frac{8\pi^2}{3\sqrt{3}a^2}.
$$

The product of these two is $A\tilde{A} = 4\pi^2$, as it should be.

*Question 3*

Solution of the Schrödinger equation (SE) in 2D, with periodic boundary conditions (PBC), yields plane–wave solutions

$$\psi(x,y) \sim e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

with allowed values of the wave vector,

$$\boldsymbol{k} = k_x\hat{x} + k_y\hat{y} = \frac{2\pi}{L}\left(n_1\hat{x} + n_2\hat{y}\right).$$

Hence, there is 1 allowed value of $\boldsymbol{k}$ in an area $(2\pi/L)^2$ in $k$–space, and, because of spin degeneracy $g_s = 2$, there are 2 allowed states within this $k$–space area. As in 3D, the DOS in $k$–space is constant,

$$D_2(\boldsymbol{k}) = \frac{2}{(2\pi/L)^2} = \frac{A}{2\pi^2}.$$

The number of states with absolute value of the wave vector smaller than a given $k$ is

$$N_2(k) = \pi k^2 \cdot \frac{A}{2\pi^2} = \frac{Ak^2}{2\pi},$$

and since $E(k) = \hbar^2 k^2/2m$, i.e., $k = \sqrt{2mE/\hbar^2}$, the number of states with energy less than $E$ is

$$N_2(E) = \frac{A}{2\pi} \cdot \frac{2mE}{\hbar^2} = \frac{mA}{\pi\hbar^2}E.$$

Therefore, the 2D DOS is

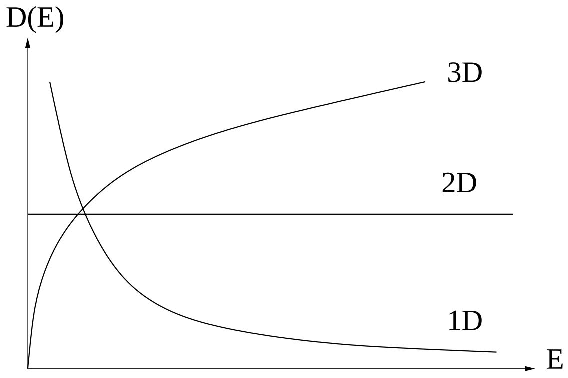
$$D_2(E) = \frac{dN_2}{dE} = \frac{mA}{\pi\hbar^2},$$

a constant, independent of the energy.

In 1D, a similar way of reasoning yields

$$\begin{aligned}
D_1(k) &= \frac{2}{2\pi/L} = \frac{L}{\pi} \\
N_1(k) &= 2k \cdot \frac{L}{\pi} = \frac{2Lk}{\pi} \\
N_1(E) &= \frac{2L}{\pi} \cdot \sqrt{2mE/\hbar^2} = \frac{2L\sqrt{2m}}{\pi\hbar}\sqrt{E} \\
D_1(E) &= \frac{dN_1}{dE} = \frac{L\sqrt{2m}}{\pi\hbar}E^{-1/2}
\end{aligned}$$

To sum up: The *dimensionality* of the system determines the energy dependence of the DOS. A qualitative sketch of the DOS in 1, 2, and 3 dimensions is given in the figure below:


D(E)
3D
2D
1D
E