Density of States in 2D

We derive the exact expression for the density of states in 2D for electrons described by the tight binding Hamiltonian $\epsilon_k = -2t(\cos k_x + \cos k_y)$. The Green's function is[87]

$$G(z) = \sum_{\mathbf{k}} \frac{|\mathbf{k}\rangle\langle\mathbf{k}|}{z - \epsilon_k} \tag{C.1}$$

in which

$$\begin{aligned} |\mathbf{k}\rangle &= \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{x}_i} |i\rangle \\ \langle i|\mathbf{k}\rangle &= e^{i\mathbf{k}\cdot\mathbf{x}_i} \end{aligned} \tag{C.2}$$

therefore

$$G_{ii}(z) = \sum_k \frac{1}{z - \epsilon_k} = \int_{1BZ} \frac{d\mathbf{k}}{z - \epsilon_k} \tag{C.3}$$

where the integration in (C.3) is over the first Brillioun zone. Now

$$\lim_{\varepsilon \to 0} \frac{1}{z - \epsilon_k} = P\left(\frac{1}{E - \epsilon_k}\right) - i\pi\delta(E - \epsilon_k) \tag{C.4}$$

where

$$z = \lim_{\varepsilon \to 0} E + i\varepsilon$$

and

$$\int_{1BZ} \delta(E - \epsilon_k) d\mathbf{k} = \int_{1BZ} d\epsilon g(\epsilon) \delta(E - \epsilon_k) = g(E) \tag{C.5}$$

hence

$$G_{ii}(z) = \int P\left(\frac{1}{E - \epsilon_k}\right) - i\pi g(E) \tag{C.6}$$

and the density of states can be written in terms of the imaginary part of the Green's function as

$$g(E) = -\frac{1}{\pi} \lim_{\varepsilon \to 0} \mathrm{Im} G_{ii}(z) \tag{C.7}$$

Now we perform the integration in (C.3)

$$G_{ii}(z) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \frac{1}{z + 2t(\cos k_x + \cos k_y)} \tag{C.8}$$

we know that

$$\cos k_x + \cos k_y = 2\cos\left(\frac{k_x + k_y}{2}\right)\cos\left(\frac{k_x - k_y}{2}\right) \tag{C.9}$$

by defining new variables $\alpha = (k_x + k_y)/2$ and $\beta = (k_x - k_y)/2$ and Eq. C.8 we have[89]

$$G_{ii}(z) = \frac{2}{(2\pi)^2} \int_{-\pi}^{\pi} d\alpha \int_{0}^{\pi} d\beta \frac{1}{z + 4t(\cos\alpha\cos\beta)} \tag{C.10}$$

also we know that (from Eq. 2.553 in Ref. [90])

$$\int \frac{dx}{a + b\cos x} = \frac{2\pi}{\sqrt{a^2 - b^2}} \tan^{-1}\left(\frac{\sqrt{a^2 - b^2}\tan(x/2)}{a + b}\right) \qquad a^2 > b^2 \tag{C.11}$$

$$\int \frac{dx}{a + b\cos x} = \frac{1}{\sqrt{b^2 - a^2}} \ln\left[\frac{\sqrt{b^2 - a^2}\tan(x/2) + (a + b)}{\sqrt{b^2 - a^2}\tan(x/2) - (a + b)}\right] \qquad a^2 < b^2 \tag{C.12}$$

so that for $a^2 > b^2$ (see :

$$\begin{aligned} G_{ii}(z) &= \frac{2\pi}{(2\pi)^2} \int_{-\pi}^{\pi} d\alpha \frac{1}{\sqrt{z^2 - 16t^2\cos^2\alpha}} \\ &= \frac{1}{\pi z} \int_0^{\pi} \frac{d\alpha}{\sqrt{1 - (4t/z)^2\cos^2\alpha}} \\ &= \frac{2}{\pi z} K(4t/z) \end{aligned} \tag{C.13}$$

where K is the elliptic integral of the first kind. For $a^2 < b^2$:

$$\int_0^{\pi} \frac{dx}{a + b\cos x} = \frac{1}{\sqrt{b^2 - a^2}} [\ln(1) - \ln(-1)] = \frac{-i\pi}{\sqrt{b^2 - a^2}} \tag{C.14}$$

therefore

$$\begin{aligned} G_{ii}(z) &= \frac{-i}{\pi} \int_0^{\pi} \frac{d\alpha}{\sqrt{(4t\cos\alpha)^2 - z^2}} \\ &= \frac{-i}{\pi 4t\sqrt{1 - (z/4t)^2}} K\left(\frac{1}{\sqrt{1 - (z/4t)^2}}\right) \end{aligned} \tag{C.15}$$

We use the relation[90]:

$$\frac{1}{q}K\left(\frac{1}{q}\right) = K(q) + iK(\sqrt{1-q^2}) \tag{C.16}$$

in which q is a complex number, therefore when $|z| < 4t$:

$$G_{ii}(E) = -\frac{i}{4t\pi}K(\sqrt{1-(E/4t)^2}) + \frac{1}{4t\pi}K(E/4t) \tag{C.17}$$

by using Eq. C.7 the density of states can be written as:

$$g(E) = \frac{\theta(E-4t)}{4\pi^2 t}K(\sqrt{1-(E/4t)^2}) \tag{C.18}$$