

**Exercise 6.1 Specific Heat of a Metal, a Semiconductor, and Graphene**

- a) The density of states for the dispersion relation  $\epsilon_{\vec{k}}$  including the spin degeneracy is given by

$$D(\epsilon) = \frac{2}{V} \sum_{\vec{k}} \delta(\epsilon - \epsilon_{\vec{k}}) = \frac{2}{(2\pi)^3} \int d^3\vec{k} \delta\left(\epsilon - \frac{\hbar^2 \vec{k}^2}{2m}\right) \quad (1)$$

where we went from a summation to an integral by approximating  $\sum_{\vec{k}} \approx V/(2\pi)^3 \int d^3\vec{k}$ . We change to spherical coordinates and get that the density of states at the Fermi energy  $\epsilon_F$  is

$$D(\epsilon_F) = \frac{8\pi}{(2\pi)^3} \int dk k^2 \delta\left(\epsilon_F - \frac{\hbar^2 k^2}{2m}\right) = \frac{1}{\pi^2} \int \underbrace{dk}_{=d(k^2)} \frac{2k}{2} \frac{\delta(2m\epsilon_F/\hbar^2 - k^2)}{\hbar^2/2m} \quad (2)$$

where we used that  $\delta(\alpha x) = \delta(x)/|\alpha|$ . Thus, we obtain

$$D(\epsilon_F) = \frac{m}{\pi^2 \hbar^2} \sqrt{\frac{2m\epsilon_F}{\hbar^2}} = \frac{mk_F}{\pi^2 \hbar^2} = \frac{3}{2} \frac{n}{\epsilon_F} \quad (3)$$

where we used  $k_F = \sqrt[3]{3\pi^2 n}$ . At  $T = 0$  the particle density and the energy density can easily be calculated since only states below the Fermi sea are occupied, i.e.

$$n = \sum_{\epsilon_{\vec{k}} < \epsilon_F} 1 \quad u = \sum_{\epsilon_{\vec{k}} < \epsilon_F} \epsilon_{\vec{k}} \quad (4)$$

but as we increase the temperature also states above the Fermi energy will be occupied. The occupation number of the states in case of Fermions is described by the Fermi-Dirac distribution function  $f_{FD}(\epsilon)$

$$f_{FD}(\epsilon) = \frac{1}{e^{(\epsilon - \mu)/k_B T} + 1}. \quad (5)$$

The particle density becomes then

$$n(\mu, T) = \sum_{\vec{k}} f_{FD}(\epsilon_{\vec{k}}) = \int d\epsilon f_{FD}(\epsilon) D(\epsilon) \quad (6)$$

and the energy density is

$$u(\mu, T) = \sum_{\vec{k}} f_{FD}(\epsilon_{\vec{k}}) \epsilon_{\vec{k}} = \int d\epsilon f_{FD}(\epsilon) D(\epsilon) \epsilon \quad (7)$$

which can be verified when you substitute  $D(\epsilon)$  using Eq. (1). In order to calculate the specific heat we need the energy density as a function of  $n$  and  $T$ . Therefore,

the goal is to invert Eq. (6) which yields  $\mu(n, T)$  and to plug it in  $u(\mu, T)$ . However, this calculation can not be done analytically. That's why we expand first Eq. (7) and (6) for small  $T$  by using the Bohr-Sommerfeld expansion, i.e. we have

$$n(\mu, T) \approx \int_0^\mu d\epsilon D(\epsilon) + \frac{\pi^2}{6} (k_B T)^2 D'(\mu) \quad (8)$$

$$u(\mu, T) \approx \int_0^\mu d\epsilon D(\epsilon)\epsilon + \frac{\pi^2}{6} (k_B T)^2 [\mu D'(\mu) + D(\mu)]. \quad (9)$$

We can use 0 as the lower integration limit, as  $D(\epsilon)$  vanishes for  $\epsilon < 0$ . Since  $\mu \rightarrow \epsilon_F$  for  $T \rightarrow 0$ , we approximate  $\int_0^\mu h(\epsilon)d\epsilon \approx \int_0^{\epsilon_F} h(\epsilon)d\epsilon + (\mu - \epsilon_F) \cdot h(\epsilon_F)$  and find then

$$\begin{aligned} n(\mu, T) &\approx \int_0^{\epsilon_F} d\epsilon D(\epsilon) + \left[ (\mu - \epsilon_F) D(\epsilon_F) + \frac{\pi^2}{6} (k_B T)^2 D'(\epsilon_F) \right] \quad (10) \\ u(\mu, T) &\approx \int_0^{\epsilon_F} d\epsilon D(\epsilon)\epsilon + \epsilon_F \left[ (\mu - \epsilon_F) D(\epsilon_F) + \frac{\pi^2}{6} (k_B T)^2 D'(\epsilon_F) \right] + \frac{\pi^2}{6} (k_B T)^2 D(\epsilon_F) \quad (11) \end{aligned}$$

where we neglected higher order contributions. If we fix the particle density, it is equal to its zero temperature value, which is the first term in Eq. (10), and therefore the expression in the brackets has to vanish. Thus, we find that

$$\mu = \epsilon_F - \frac{\pi^2}{6} (k_B T)^2 \frac{D'(\epsilon_F)}{D(\epsilon_F)} = \epsilon_F \left[ 1 - \frac{1}{3} \left( \frac{\pi k_B T}{2\epsilon_F} \right)^2 \right]. \quad (12)$$

Combining Eq. (12) with Eq. (11) we can get rid of  $\mu$  and obtain

$$u(n, T) = u_0 + \frac{\pi^2}{6} (k_B T)^2 D(\epsilon_F) \quad (13)$$

with a temperature independent energy offset  $u_0$ . Finally, the specific heat is given by

$$c_v = \left( \frac{\partial u}{\partial T} \right)_n = \frac{\pi^2}{3} k_B^2 T D(\epsilon_F) = \frac{\pi^2}{2} \left( \frac{k_B T}{\epsilon_F} \right) n k_B \quad (14)$$

where we used Eq. (3).

- b) We assume that, for  $k_B T \ll E_g$ , only the band edges are important and parametrize the dispersion by effective masses,

$$\varepsilon_v(k) = -\frac{\hbar^2 k^2}{2m_v}, \quad (15)$$

$$\varepsilon_c(k) = E_g + \frac{\hbar^2 k^2}{2m_c}. \quad (16)$$

It is a matter of convention to define the zero in energy to the upper band edge of the valence band. Instead, we could have also measured the energy with respect to the middle of the band gap.

The number of electrons must be equal to the number of holes. This enables us to determine the chemical potential through

$$0 = \int_{\text{BZ}} \frac{d^3k}{4\pi^3} \{1 - n_F[\varepsilon_v(k)]\} - \int_{\text{BZ}} \frac{d^3k}{4\pi^3} n_F[\varepsilon_c(k)] \quad (17)$$

$$= \int_{\text{BZ}} \frac{d^3k}{4\pi^3} \left\{ \frac{1}{e^{-[\varepsilon_v(k)-\mu]/k_B T} + 1} - \frac{1}{e^{[\varepsilon_c(k)-\mu]/k_B T} + 1} \right\} \quad (18)$$

$$\approx \int_{\text{BZ}} \frac{d^3k}{4\pi^3} \{e^{[\varepsilon_v(k)-\mu]/k_B T} - e^{-[\varepsilon_c(k)-\mu]/k_B T}\}, \quad (19)$$

where, in the last step, we have assumed  $\mu \gg k_B T$  and  $E_g - \mu \gg k_B T$ , which gives

$$\frac{1}{e^{\epsilon/k_B T} + 1} \approx e^{-\epsilon/k_B T}, \quad (20)$$

with  $\epsilon \gg k_B T$ . Note that this corresponds to using Maxwell-Boltzmann statistics as for the ideal gas, rather than the Fermi-Dirac statistics.

From the equation (19) we find

$$0 = \frac{(2k_B T)^{3/2}}{4\pi^3 \hbar^3} \left( \int_{\mathbb{R}^3} d^3y e^{-y^2} \right) \{m_v^{3/2} e^{-\mu/k_B T} - m_c^{3/2} e^{(\mu-E_g)/k_B T}\}, \quad (21)$$

where we have used the fact that the Gaussian integral converges very rapidly so that we can extend the integral over the first Brillouin zone to an integral over  $\mathbb{R}^3$ .

The first two factors in the last equation are strict positive, so the last factor must vanish to fulfill the equation. Hence we find

$$\mu = \frac{E_g}{2} + \frac{3}{4} k_B T \log \left( \frac{m_v}{m_c} \right). \quad (22)$$

For  $T = 0$ , the chemical potential is in the middle of the band gap.

We first calculate the number of excited electrons  $n_e(T)$ , which is equal to the number of holes, where we again can extend the region of integration from the first Brillouin zone to the entire real space in order to perform Gaussian integration.

$$n_h(T) = \int_{\text{BZ}} \frac{d^3k}{4\pi^3} \{1 - n_F[\varepsilon_v(k)]\} \approx \int_{\text{BZ}} \frac{d^3k}{4\pi^3} e^{[\varepsilon_v(k)-\mu]/k_B T} \quad (23)$$

$$= e^{-\mu/k_B T} \left( \frac{m_v k_B T}{2^{1/3} \pi \hbar^2} \right)^{3/2} = \left( \frac{k_B T}{2^{1/3} \pi \hbar^2} \right)^{3/2} (m_v m_c)^{3/4} e^{-E_g/2k_B T}. \quad (24)$$

In the last step, we have inserted  $\mu$  from Eq. (22).

Next, we calculate the total energy of electrons and holes

$$\begin{aligned} E_v &= \int_{\text{BZ}} \frac{d^3k}{4\pi^3} [-\varepsilon_v(k)] \{1 - n_F[\varepsilon_v(k)]\} \approx \int_{\text{BZ}} \frac{d^3k}{4\pi^3} \frac{\hbar^2 k^2}{2m_v} e^{[\varepsilon_v(k) - \mu]/k_B T} \\ &= \frac{3}{2} \left( \frac{k_B T}{2^{1/3} \pi \hbar^2} \right)^{3/2} (m_v m_c)^{3/4} e^{-E_g/2k_B T} k_B T = \frac{3}{2} n_h(T) k_B T, \end{aligned} \quad (25)$$

$$\begin{aligned} E_c &= \int_{\text{BZ}} \frac{d^3k}{4\pi^3} \varepsilon_c(k) n_F[\varepsilon_c(k)] \approx \int_{\text{BZ}} \frac{d^3k}{4\pi^3} \left( \frac{\hbar^2 k^2}{2m_v} + E_g \right) e^{[\mu - \varepsilon_c(k)]/k_B T} \\ &= \left( \frac{3}{2} k_B T + E_g \right) \left( \frac{k_B T}{2^{1/3} \pi \hbar^2} \right)^{3/2} (m_v m_c)^{3/4} e^{-E_g/2k_B T} = \left( \frac{3}{2} k_B T + E_g \right) n_e(T). \end{aligned} \quad (26)$$

Note that the energy of holes enters Eq. (25) with the negative value of the energy of the electrons in the valence band,  $-\varepsilon_v(k)$ .

In total, we have

$$E = n(T) \left[ \frac{3}{2} k_B T + \frac{E_g}{2} \right], \quad (27)$$

with the total number of carriers  $n(T) = n_e(T) + n_h(T)$ .

The specific heat is thus given by a ideal gas-like part plus a correction,

$$C = \frac{3}{2} n(T) k_B + \left[ \frac{3}{2} k_B T + \frac{E_g}{2} \right] \frac{\partial n(T)}{\partial T}. \quad (28)$$

We see that the specific heat of a semiconductor is given by a contribution similar to the specific heat of an ideal gas of excitations that are already present in the system due to thermal excitation, plus an additional contribution originating from the excitation of new particle hole pairs  $\sim \frac{\partial n(T)}{\partial T}$ .

Given that

$$\frac{\partial n(T)}{\partial T} = \left( \frac{3}{2} + \frac{E_g}{2k_B T} \right) \frac{n(T)}{T}, \quad (29)$$

we can rewrite the specific heat as

$$C = \left[ \frac{15}{4} k_B + \frac{E_g}{T} \left( \frac{3}{2} + \frac{E_g}{4k_B T} \right) \right] n(T). \quad (30)$$

Thus, the part of the specific heat originating from the excitation of additional particles dominates over the ideal gas-like part for small temperatures!

- c) We first consider the chemical potential. For this we use a two-band approximation (like a semiconductor with the gap going to zero) and find for the number of electrons and holes

$$n_e = c \int d^2k f_{FD}(\epsilon_c) = c \int d^2k \frac{1}{e^{\beta(\hbar v_F |k| - \mu)} + 1} \quad (31)$$

$$n_h = 1 - n_v = c \int d^2k (1 - f_{FD}(\epsilon_v)) = c \int d^2k \frac{1}{e^{-\beta(-\hbar v_F |k| - \mu)} + 1}, \quad (32)$$

where  $c$  takes care of the volume in reciprocal space and the degeneracies. Since  $n_e \stackrel{!}{=} n_h$  we have

$$\int d^2k \frac{1}{e^{\beta(\hbar v_F |k| - \mu)} + 1} \stackrel{!}{=} \int d^2k \frac{1}{e^{\beta(\hbar v_F |k| + \mu)} + 1}, \quad (33)$$

from which it follows immediately that

$$\mu = 0 \forall T. \quad (34)$$

For the density of states we have as above

$$D(\epsilon) = \frac{2 \cdot 2}{A} \sum_{\vec{k}} \delta(\epsilon - \epsilon_{\vec{k}}), \quad (35)$$

where the spins lead to a degeneracy of 2 and the two equivalent Dirac points to another degeneracy of 2 (valley degeneracy). Due to the symmetry about the Dirac point it is enough to consider the case  $\epsilon > 0$ . Again, we replace the sum by an integral and find

$$D(\epsilon) = \frac{4}{(2\pi)^2} \int d^2k \delta(\epsilon - \epsilon_{\vec{k}}) \quad (36)$$

$$= \frac{2}{\pi} \int_0^\infty k dk \delta(\epsilon - \hbar v_F k) \quad (37)$$

$$= \frac{2}{\pi \hbar v_F} \int_0^\infty k dk \delta\left(\frac{\epsilon}{\hbar v_F} - k\right). \quad (38)$$

Therefore

$$D(\epsilon) = \frac{2}{\pi (\hbar v_F)^2} |\epsilon|, \quad (39)$$

which is linear in the energy.

We also evaluate the number of electrons which is equal to the number of holes

$$n_e(T) = 4 \int \frac{d^2k}{(2\pi)^2} f_{FD}(\epsilon_c) = \int \frac{d^2k}{\pi^2} \frac{1}{e^{\beta(\hbar v_F |k| - \mu)} + 1} \quad (40)$$

$$= \frac{2}{\pi} \int_0^\infty dk k \frac{1}{e^{\beta \hbar v_F k} + 1} \quad (41)$$

$$= \frac{2}{\pi (\beta \hbar v_F)^2} \int_0^\infty dk \frac{k}{e^k + 1} \quad (42)$$

$$= \frac{2}{\pi (\beta \hbar v_F)^2} \frac{\pi^2}{12} = \frac{\pi}{6 (\hbar v_F)^2} (k_B T)^2 = n_h(T). \quad (43)$$

We are ready to evaluate the internal energy  $u$  and find

$$u(T) - u_0 = \int d\epsilon f_{FD}(\epsilon) D(\epsilon) \epsilon - u_0 \quad (44)$$

$$= \frac{2}{\pi(\hbar v_F)^2} \left( \int d\epsilon \frac{\epsilon|\epsilon|}{e^{\beta(\epsilon-\mu)} + 1} - \int_{-\infty}^{\epsilon_F} d\epsilon \epsilon|\epsilon| \right) \quad (45)$$

$$= \frac{2}{\pi(\hbar v_F)^2} \left( \int_0^\infty d\epsilon \frac{\epsilon^2}{e^{\beta\epsilon} + 1} + \int_{-\infty}^0 d\epsilon \frac{-\epsilon^2}{e^{\beta\epsilon} + 1} + \int_{-\infty}^0 d\epsilon \epsilon^2 \right) \quad (46)$$

$$= \frac{2}{\pi(\hbar v_F)^2} \left( \int_0^\infty d\epsilon \frac{\epsilon^2}{e^{\beta\epsilon} + 1} + \int_{-\infty}^0 d\epsilon \frac{\epsilon^2}{e^{-\beta\epsilon} + 1} \right) \quad (47)$$

$$= \frac{4}{\pi(\hbar v_F)^2 \beta^3} \int_0^\infty dx \frac{x^2}{e^x + 1} \quad (48)$$

$$= \frac{4(k_B T)^3}{\pi(\hbar v_F)^2} \frac{3}{2} \zeta(3). \quad (49)$$

Therefore the specific heat is given by

$$c = \left. \frac{\partial u}{\partial T} \right|_n = \frac{18\zeta(3)k_B}{\pi(\hbar v_F)^2} (k_B T)^2. \quad (50)$$

## Exercise 6.2 Spin Susceptibility of a Metal, a Semiconductor, and Graphene

- a) An external magnetic field  $H$  coupling to the electron spins  $s = \pm 1$  (neglecting any orbital effects) changes the energy according to

$$\epsilon_{\vec{k},s} = \epsilon_{\vec{k}} - \mu_B s H, \quad (51)$$

where  $\mu_B$  is the Bohr magneton. There are now two distinct Fermi-Dirac distributions and the number of electrons in each spin state is given by

$$n_s(H) = \int d\epsilon \frac{1}{2} D(\epsilon) f_{FD}(\epsilon_{\vec{k},s}). \quad (52)$$

With the magnetization defined as

$$M = \mu_B (n_+ - n_-), \quad (53)$$

we immediately find

$$M = \mu_B \int d\epsilon \frac{1}{2} D(\epsilon) (f_{FD}(\epsilon - \mu_B H) - f_{FD}(\epsilon + \mu_B H)) \quad (54)$$

$$\approx \mu_B^2 H \int d\epsilon D(\epsilon) \left( -\frac{\partial f_{FD}}{\partial \epsilon} \right) \quad (55)$$

$$\approx \mu_B^2 H D(\epsilon_F). \quad (56)$$

Then the Pauli spin susceptibility is given by

$$\chi_{Pauli} = \left. \frac{\partial M}{\partial H} \right|_{H=0} = \mu_B^2 D(\epsilon_F), \quad (57)$$

which is temperature independent.

b) As for the metal, we have

$$M \approx \mu_B^2 H \int d\epsilon D(\epsilon) \left( -\frac{\partial f_{FD}}{\partial \epsilon} \right). \quad (58)$$

For the semiconductor, however, we have to be more careful with the derivative because of the gap.

Neglecting excitons and other interactions, we simply model the semiconductor as a paramagnetic ideal gas. Both the electron and the hole system are unpolarized at zero applied field (same number of up and down spins in the thermally excited electrons) and their contribution to the magnetization is the same,  $M_{tot} = M_h + M_e$ . Again using the approximation of  $\epsilon \gg k_b T$ , we write for the electrons in the conduction band

$$M_e \approx \mu_B^2 H \int \frac{d^3 k}{4\pi^3} \frac{\beta e^{\beta(\epsilon_c - \mu)}}{(e^{\beta(\epsilon_c - \mu)} + 1)^2} \quad (59)$$

$$= \mu_B^2 H \beta \int \frac{d^3 k}{4\pi^3} e^{-\beta(\epsilon_c - \mu)}. \quad (60)$$

But this is exactly the integral we had before for the number of electrons. Using  $n(T) = n_h(T) = n_e(T)$  we can write immediately

$$M_{tot} = (M_h + M_e) \approx \mu_B^2 H \beta n(T) \quad (61)$$

which gives

$$\chi_{Pauli} = \frac{\mu_B^2}{k_B} \frac{n(T)}{T}. \quad (62)$$

This is like Curie's law, reflecting the ideal gas behavior of the semiconductor. However, the particle density  $n(T)$  is temperature dependent and decays exponentially at low temperatures.

The major contribution to the susceptibility in semiconductors stems from the diamagnetism of the ion cores. However, in doped semiconductors, the conduction electron diamagnetism can be dominant.

c) Again we start with

$$M \approx \mu_B^2 H \int d\epsilon D(\epsilon) \left( -\frac{\partial f_{FD}}{\partial \epsilon} \right). \quad (63)$$

We use a two-band approach, where we only have to calculate the contribution from the electrons in the conduction band, because  $M_h = M_e$  as for the semiconductor. We find

$$M_e \approx \mu_B^2 H \frac{2}{\pi(\hbar v_F)^2} \int_0^\infty d\epsilon \epsilon \frac{\beta e^{\beta\epsilon}}{(e^{\beta\epsilon} + 1)^2} \quad (64)$$

$$= \mu_B^2 H \frac{2}{\pi(\hbar v_F)^2 \beta} \int_0^\infty d\epsilon \frac{\epsilon e^{\beta\epsilon}}{(e^\epsilon + 1)^2} \quad (65)$$

$$= \mu_B^2 H \frac{2}{\pi(\hbar v_F)^2 \beta} \int_0^\infty d\epsilon \frac{\epsilon}{\cosh^2 \epsilon} \quad (66)$$

$$= \mu_B^2 H \frac{2}{\pi(\hbar v_F)^2 \beta} \log 2. \quad (67)$$

The total Pauli spin susceptibility is then given by

$$\chi_{Pauli} = \mu_B^2 \frac{4 \log 2}{\pi (\hbar v_F)^2} k_B T. \quad (68)$$

Note that in real graphene, the susceptibility due to Landau diamagnetism of free electrons and holes is dominant.

### Exercise 6.3 Density of States from the Tight-Binding Model

Setting  $a = 1$ , we have in  $d$  dimensions

$$D(\epsilon) = \frac{2}{L^d} \sum_{\vec{k}} \delta(\epsilon - \epsilon_{\vec{k}}) = \frac{2}{L^d} \sum_{k_i} \delta\left(\epsilon + 2t \sum_i \cos k_i\right). \quad (69)$$

We see that  $D(\epsilon)$  is only defined for  $|\frac{\epsilon}{2t}| \leq d$ , and it is symmetric  $D(+\epsilon) = D(-\epsilon)$ . In 1d we find analytically

$$\begin{aligned} D(\epsilon) &= \frac{2}{L} \sum_{\vec{k}} \delta(\epsilon - \epsilon_{\vec{k}}) = \frac{2}{2\pi} \int_{-\pi}^{\pi} dk \delta(\epsilon + 2t \cos k) \\ &= \frac{2}{2\pi} \frac{2}{2t} \int_0^{\pi} dk \delta\left(\frac{\epsilon}{2t} + \cos k\right) = \frac{1}{\pi t} \int_{-1}^1 \frac{dy}{\sqrt{1-y^2}} \delta\left(\frac{\epsilon}{2t} + y\right) = \frac{1}{\pi t \sqrt{1 - \left(\frac{\epsilon}{2t}\right)^2}}. \end{aligned} \quad (70)$$

In higher dimensions we use numerics. We approximate the  $\delta$ -function as

$$\delta(x; \delta) \approx \frac{\delta}{\pi(x^2 + \delta^2)}. \quad (71)$$

For  $N$  lattice points we write using symmetry considerations

$$D(\epsilon) = \frac{2}{N^d} \frac{1}{2t} \sum_{\substack{k_i = -\pi, \\ \Delta k_i = 2\pi/N}}^{\pi} \delta\left(\frac{\epsilon}{2t} + \sum_i \cos k_i\right) = \frac{2}{(N/2)^d} \frac{1}{2t} \sum_{\substack{k_i = 0, \\ \Delta k_i = 2\pi/N}}^{\pi} \delta\left(\frac{\epsilon}{2t} + \sum_i \cos k_i\right), \quad (72)$$

where we used that  $L = Na$  with  $a = 1$  and changed the bounds in the sum.

In Fig. 1 we plot the numerical result for 1d, 2d and 3d, together with the analytical result in 1d and in Fig. 2 we show the code.

We encounter the van Hove singularities in all dimensions: in 1d there is a square-root divergence at the edges, in 2d there is a logarithmic divergence in the center and in 3d there is an infinite slope at the edges and a kink near  $1/3$ . Their nature becomes apparent when considering an alternate way of writing the density of states (see for example Ashcroft&Mermin )

$$D(\epsilon) = \frac{2}{(2\pi)^d} \int_{S(\epsilon)} dS \frac{1}{|\nabla \epsilon(\vec{k})|}, \quad (73)$$

where the surface integral is over  $S(\epsilon)$ , which is a surface of constant energy ( $\epsilon(\vec{k}) \equiv \epsilon$ ). The van Hove singularities appear whenever  $|\nabla \epsilon(\vec{k})| = 0$ .



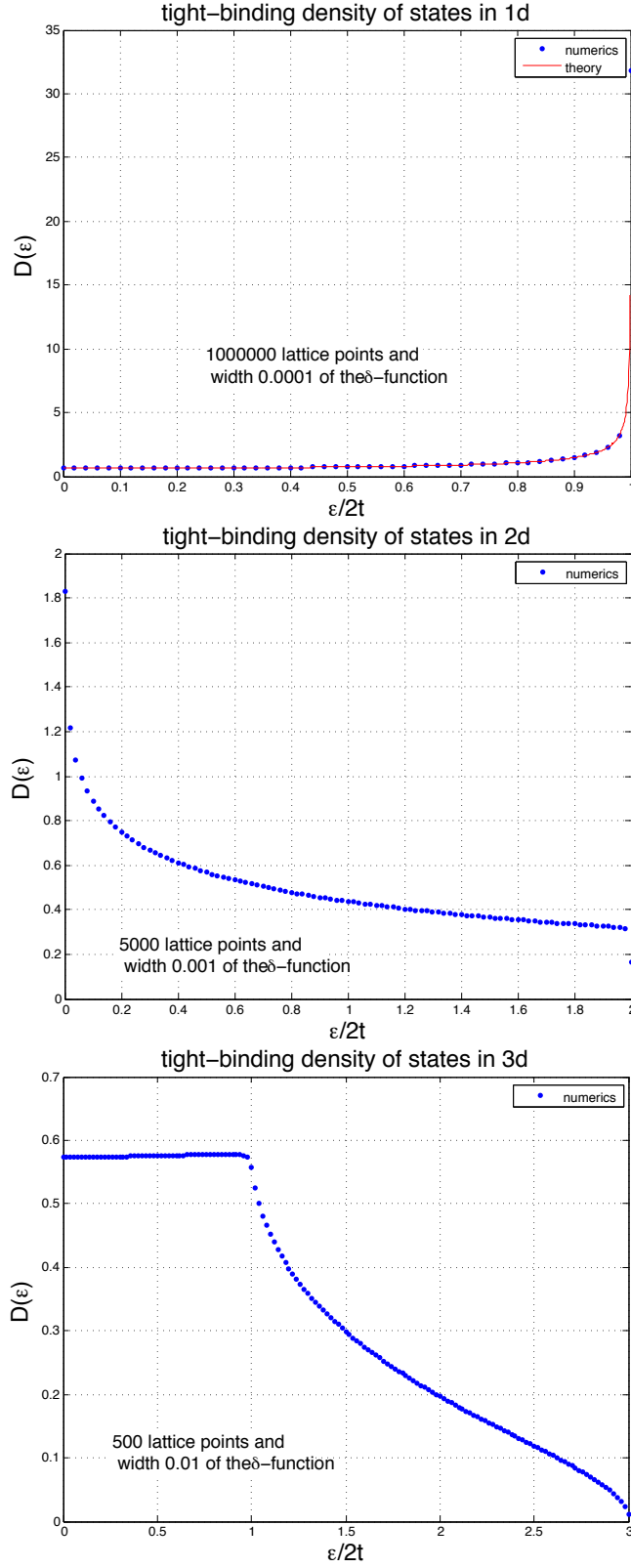


Figure 1: The density of states in the tight binding model for 1d, 2d and 3d calculated numerically and compared to the analytical result for 1d. We set  $t = 0.5$ .

```

1 function tb_dos_plot(dim,m,n,d)
2 %plots the density of states  $D(e)$  with a mesh of step size  $1/m$  in  $e$ 
3 %using  $n$  lattice points and width  $d$  in the delta function
4
5 for e=1:(dim*m+1)
6     tb_dos(e)=tb_dos_sum(dim,(e-1)/m,n,d);
7 end
8 plot((0:1/m:dim),tb_dos, '.')
9 grid on
10 title(sprintf('tight-binding density of states in %dd',dim),'FontSize',18)
11 ylabel('D(\epsilon)','FontSize',18)
12 xlabel('\epsilon/2t','FontSize',18)
13 legend('numerics','FontSize',14)
14 text(0.25,0.25,sprintf('%d lattice points and\n width %g of the\delta-function',n,d),
    'BackgroundColor',[1 1 1],'FontSize',14,'Units','normalized')
15
16 function [s_out] = tb_dos_sum(dim,e,n,d)
17 %computes the density of states  $D(e)$  for one specific  $e$ 
18 %using  $n$  lattice points and width  $d$  in the delta function
19
20 s=0;
21
22 if(dim==1)
23     for kx=0:(2*pi/n):pi
24         s=s+d/(pi*((e+cos(kx))^2+d^2));
25     end
26
27 elseif(dim==2)
28     for kx=0:(2*pi/n):pi
29         for ky=0:(2*pi/n):pi
30             s=s+d/(pi*((e+cos(kx)+cos(ky))^2+d^2));
31         end
32     end
33
34 elseif(dim==3)
35     for kx=0:(2*pi/n):pi
36         for ky=0:(2*pi/n):pi
37             for kz=0:(2*pi/n):pi
38                 s=s+d/(pi*((e+cos(kx)+cos(ky)+cos(kz))^2+d^2));
39             end
40         end
41     end
42
43 end
44
45 s_out=2*s/(n/2)^dim;

```

Figure 2: The Matlab code to generate the above figures