



FY2045 Solutions Problem set 7 fall 2023

Professor Jens O. Andersen and Henning G. Hugdal

December 11, 2023

Problem 1

- a) The energies of a state is given in terms of the three positive integers n_x , n_y , and n_z ,

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2 + n_z^2}{L^2} \right). \quad (1)$$

In the expression for the energy, it is important to distinguish between the edges L in the y - and z -directions (which are kept fixed) and L_x , which varies. If we allow the piston to move, corresponding to an infinitesimal increase dL_x of L_x , with $L_y = L_z = L$ kept fixed, the particle does the work $F_x dL_x$ on the piston. This work is taken from the energy of the particle. Therefore we must have

$$F_x dL_x = -dE. \quad (2)$$

Thus the force on the piston is

$$F_x = -\frac{\partial E}{\partial L_x} = \frac{\hbar^2 \pi^2 n_x^2}{m L_x^3} = \frac{\hbar^2 \pi^2}{\underline{\underline{m L_x^3}}}, \quad (3)$$

since $n_x = 1$ for ground state. We see that the force is inversely proportional to the mass m of the particle. The force vanishes in the macroscopic limit, that is, $m \rightarrow \infty$. This agrees with classical mechanics, where the ground state corresponds to the particle being at rest. In the opposite limit, we see that the force increases with decreasing mass. The same goes for the energy of the ground state.

b) Taking spin into account the 8 spin- $\frac{1}{2}$ fermions in the ground state form four pairs that occupy the four spatial one-particle states with the lowest one-particle energies. When L_x is close to L , the quantum numbers of these four spatial states are given by ¹

$$(n_x, n_y, n_z) = (1, 1, 1), (2, 1, 1), (1, 2, 1), \text{ and } (1, 1, 2) . \quad (4)$$

The force depends only on the L_x -dependent contributions to the total energy of the eight particles, which are

$$E_{\text{tot}}^{(x)} = \frac{\hbar^2 \pi^2}{2m} 2 \left(\frac{1}{L_x^2} + \frac{4}{L_x^2} + \frac{1}{L_x^2} + \frac{1}{L_x^2} \right) = 7 \frac{\hbar^2 \pi^2}{m L_x^2} . \quad (5)$$

For $L_x = L$, the force then is

$$F_x = - \left. \frac{\partial E_{\text{tot}}^{(x)}}{\partial L_x} \right|_L = 14 \frac{\hbar^2 \pi^2}{m L^3} . \quad (6)$$

Thus, the force from the 8 identical fermions, when they are in the ground state, is 14 times larger than with only one such particle present.

Problem 2

a) The periodic boundary condition in the x -direction is $\psi(0, y) = \psi(L, y)$, which implies

$$1 = e^{ik_x L} . \quad (7)$$

Writing $1 = e^{2n\pi i}$ and taking the logarithm on both sides, yields the allowed values for $p = \hbar k$,

$$p_x = \frac{2\pi \hbar n_x}{L} , \quad (8)$$

where $n_x \in \mathbb{Z}$. The same argument applies in the y -direction such that $p_y = \frac{2\pi \hbar n_y}{L}$ and $n_y \in \mathbb{Z}$.

The number of states inside a circle of radius $R = \sqrt{n_x^2 + n_y^2}$ is

$$\begin{aligned} N &= \pi R^2 \\ &= \pi(n_x^2 + n_y^2) . \end{aligned} \quad (9)$$

Note that we take into account the whole circle and not only the quarter in the first quadrant due to the fact that $n_x, n_y \in \mathbb{Z}$ and not \mathbb{N} . Expressing this in terms of the momenta yields

$$N = \pi \frac{L^2}{4\pi^2 \hbar^2} (p_x^2 + p_y^2) = \frac{L^2}{4\pi \hbar^2} p^2 , \quad (10)$$

¹Note that the quantum numbers of the four lowest-lying states depend on L_x : If e.g. $L_x \ll L$, then all four of the states will have $n_x = 1$. On the other hand, if $L_x \gg L$, then all four will have $n_y = n_z = 1$.

where $p = \sqrt{p_x^2 + p_y^2}$ is the magnitude of the momentum. The density of states $g(p)$ is $\frac{dN}{dp}$, which yields

$$g(p) = \frac{L^2}{\underline{\underline{2\pi\hbar^2}}} p. \quad (11)$$

or

$$g(p)dp = \frac{L^2}{(2\pi\hbar)^2} d^2p, \quad (12)$$

where we have used $d^2p = 2\pi p dp$ in polar coordinates in two dimensions.² This is in contrast to the constant density of states $g(\mathbf{p}) = \left(\frac{L}{2\pi\hbar}\right)^2$ (or $g(\mathbf{k}) = \left(\frac{L}{2\pi}\right)^2$) derived in class: Each state in p -space occupies a volume $(2\pi\hbar/L)^2$ corresponding to a pair of indexes (n_x, n_y) . However, in 2D,³ multiple states can have the same momentum magnitude, and the number of possible combinations of momenta giving the same magnitude increases as the momentum increases, resulting in a density of states $g(p) \propto p$. In higher dimensions the increase is even more rapid, resulting in higher powers of p .

b) In the infinite-volume limit, the sum over states is then replaced by an integral according to the rule

$$\sum_n \rightarrow (\text{Volume in } p\text{-space}) \times (\text{Density of states in } p\text{-space}) = \frac{L^2}{\hbar^2} \int \frac{d^2p}{(2\pi)^2}. \quad (13)$$

We can limit the integration area in p -space to values of $p \equiv |\mathbf{p}| < p_F$ by inserting a Heaviside step function $\theta(p_F - p)$ in the integral.

The particle density reads (factor two due to spin)⁴

$$\begin{aligned} \rho = \frac{N}{V} &= \frac{2}{\hbar^2} \int \frac{d^2p}{(2\pi)^2} \theta(p_F - p) = \frac{1}{\pi\hbar^2} \int_0^{p_F} dp \, p \\ &= \frac{1}{\underline{\underline{2\pi\hbar^2}}} p_F^2, \end{aligned} \quad (14)$$

²To see how this comes about, we define the momenta in polar coordinates, $p_x = p \cos \phi$ and $p_y = p \sin \phi$, and express the integration over a circular area in p -space in terms of these coordinates:

$$\int_{\text{circ}} d^2p \, f(\mathbf{p}) = \int_{\text{circ}} dp_x dp_y \, f(p_x, p_y) = \int_0^{2\pi} d\phi \int dp \, p f(p, \phi).$$

If the function we integrate over does not depend on the angle ϕ , this simplifies to $\int d^2p \, f(p) = 2\pi \int dp \, p f(p)$, meaning we can write the integration measure as $d^2p = 2\pi p dp$ in polar coordinates when integrating over a radially symmetric function.

³In fact for any spatial dimension above 1D.

⁴One can use a step function with argument $E_F - E$ as well.

with the 2D volume (i.e. area) $V = L^2$. Notice that this is exactly the same as what we would get if we had used the expression for N in eq. (10) with $p = p_F$ and accounting for spin.

The energy density reads

$$\mathcal{E} = \frac{E_{\text{tot}}}{V} = \frac{2}{\hbar^2} \int \frac{d^2 p}{(2\pi)^2} \sqrt{m^2 c^4 + p^2 c^2} \theta(p_F - p)$$

Performing the integral, we get

$$\mathcal{E} = \frac{m^3 c^4}{3\pi \hbar^2} \left[(1 + x_F^2)^{\frac{3}{2}} - 1 \right], \quad (15)$$

where $x_F = \frac{p_F}{mc}$. Finally, the pressure is given by

$$P = - \frac{\partial E_{\text{tot}}}{\partial V} = - \frac{\partial(\mathcal{E}V)}{\partial V} = -\mathcal{E} - V \frac{\partial \mathcal{E}}{\partial V} = -\mathcal{E} - V \frac{\partial \mathcal{E}}{\partial x_F} \frac{\partial x_F}{\partial V}.$$

It is not immediately clear why x_F should depend on V at all, giving a non-zero partial derivative with respect to V . However, from eq. (14), we see that $p_F = \sqrt{2\pi \hbar^2 \rho} = \sqrt{2\pi \hbar^2 N/V}$ depends on V , which when using $x_F = p_F/(mc)$ results in

$$\frac{\partial x_F}{\partial V} = \frac{1}{mc} \frac{\partial p_F}{\partial V} = -\frac{p_F}{2mcV} = -\frac{x_F}{2V}.$$

Combined with

$$\frac{\partial \mathcal{E}}{\partial x_F} = \left[\frac{m^3 c^4}{\pi \hbar^2} x_F \sqrt{1 + x_F^2} \right],$$

we therefore get

$$\begin{aligned} P &= -\mathcal{E} - V \left(-\frac{x_F}{2V} \right) \left[\frac{m^3 c^4}{\pi \hbar^2} x_F \sqrt{1 + x_F^2} \right] \\ &= -\frac{m^3 c^4}{6\pi \hbar^2} \left[2(1 + x_F^2) \sqrt{1 + x_F^2} - 2 \right] + 3 \frac{m^3 c^4}{6\pi \hbar^2} x_F^2 \sqrt{1 + x_F^2} \\ &= \frac{m^3 c^4}{6\pi \hbar^2} \left[(x_F^2 - 2) \sqrt{1 + x_F^2} + 2 \right]. \end{aligned} \quad (16)$$

c) The ultrarelativistic limit is obtained by taking the limit $m \rightarrow 0$. This yields

$$\mathcal{E} = \frac{c}{3\pi \hbar^2} p_F^3, \quad (17)$$

$$P = \frac{c}{6\pi \hbar^2} p_F^3. \quad (18)$$

Substituting $p_F = \sqrt{2\pi\hbar^2\rho}^{\frac{1}{2}}$ into Eq. (18), we obtain

$$P = \frac{\sqrt{2\pi c\hbar}}{3}\rho^{\frac{3}{2}}. \quad (19)$$

Note that $P = \frac{1}{2}\mathcal{E}$ in two dimensions as compared to $P = \frac{1}{3}\mathcal{E}$ in three dimensions. In the nonrelativistic limit, we expand around $x_F = 0$. To second order, we obtain

$$\begin{aligned} \mathcal{E} &= \frac{m^3 c^4}{3\pi\hbar^2} \left[\frac{3}{2}x_F^2 + \frac{3}{8}x_F^4 + \dots \right] \\ &= mc^2 \frac{p_F^2}{2\pi\hbar^2} + \frac{p_F^4}{8\pi\hbar^2 m} \\ &= \underline{\underline{mc^2\rho + \frac{\pi\hbar^2}{m}\rho^2}}. \end{aligned} \quad (20)$$

The first term is simply the rest-mass energy density, while the second term results from using the relation $E = \frac{p^2}{2m}$. The pressure is obtained in the same manner and reads

$$\begin{aligned} P &= \frac{m^3 c^4}{6\pi\hbar^2} \frac{3}{4}x_F^4 \\ &= \frac{p_F^4}{8\pi\hbar^2 m} \\ &= \underline{\underline{\frac{\pi\hbar^2}{m}\rho^2}}. \end{aligned} \quad (21)$$

If we ignore the rest-mass energy density, we have $P = \mathcal{E}$ in two dimensions, in contrast to $P = \frac{2}{3}\mathcal{E}$ in three dimensions.

Problem 3

a) The wavenumbers are quantized according to $k_i = 2\pi n_i/L_i$ with $n_i \in \mathbb{Z}$, and the energy is given by

$$E(\mathbf{k}) = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2). \quad (22)$$

In the macroscopic limit, i.e. we have large $V = L_x L_y L_z$, we can treat the states as lying very close together, forming a continuum of states. To make the numerical calculations easier to handle, we will define dimensionless wavenumbers $\kappa_i = (L_x L_y L_z)^{1/3} k_i$, such that the energy becomes

$$E(\boldsymbol{\kappa}) = \frac{\hbar^2}{2mV^{2/3}}(\kappa_x^2 + \kappa_y^2 + \kappa_z^2) \equiv E_0(\kappa_x^2 + \kappa_y^2 + \kappa_z^2), \quad (23)$$

where we have defined the constant $E_0 = \hbar^2/(2mV^{2/3})$ with units of energy. For simplicity, we set $E_0 = 1$ (this is just the same as saying that we use E_0 as our energy unit), and look at $\kappa_i \in (-1, 1)$ in the numerical calculations. See the attached code for one suggested way of calculating the density of states numerically. The results should look something like Fig. 1.

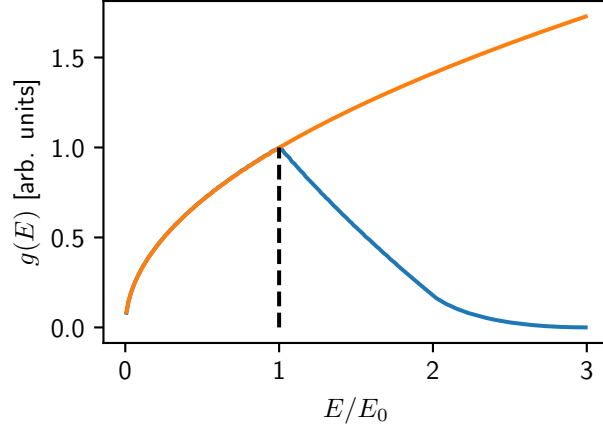


Figure 1: Numerically calculated DOS (blue) and analytical result (orange). The dashed line indicates $E = 1$, above which not all energy states are included in the calculation, resulting in a reduced DOS compared to the analytical result.

The reason the results do not agree for high energies is that along or close to the diagonals in k -space we get states of higher energy than we include along the x/y -axes — they lie outside a sphere with radius $|\kappa| = 1$, corresponding to $E = 1$ in the figure. If we had simply increased the range of κ_i , we would move this region to still higher energies.

b) Calculating the DOS for the different spatial dimensions and energy expressions, gives the results shown in Fig. 2. The density of states is constant when $d/n - 1 = 0$. This can be shown analytically as well. We have

$$E \propto k^n \quad \Rightarrow \quad k \propto E^{1/n}, \quad (24)$$

which allows us to calculate the total number of particles with energy less than E ,

$$\begin{aligned} N &= (\text{Volume in } k\text{-space}) \times (\text{Density of states in } k\text{-space}) \\ &\propto k^d \times (\text{constant}) \propto E^{d/n}. \end{aligned} \quad (25)$$

The density of states thus becomes

$$g(E) = \frac{dN}{dE} \propto E^{\frac{d}{n}-1}. \quad (26)$$

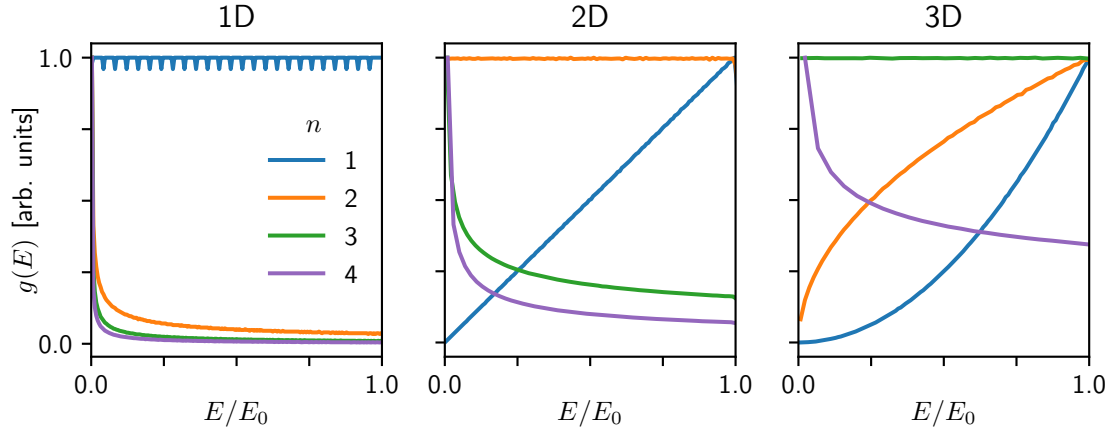


Figure 2: DOS for different n for $d = 1 - 3$ (left to right). We see that the density of states is constant if $d/n = 1$, though the numerical error is quite significant in the 1D case. Notice also that the DOS diverges for low energies if $n > d$.

We may also notice something else: when $n > d$, the DOS diverges at low E . Why do you think that is?

c) From the plot in Fig. 3, we see the density of states has a divergence at $E = 0$.

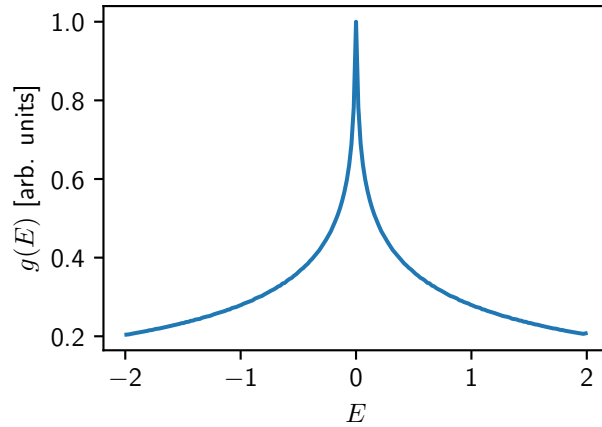


Figure 3: Density of states for the 2D tight binding model, which diverges at $E = 0$.

```

1  """
2  Suggested solution to problem set 7, FY2045 Quantum Mechanics I
3
4  By Henning G. Hugdal
5
6  Sep. 12, 2022, updated Oct. 12, 2023.
7  """
8
9  # Imports and plot edits
10 import numpy as np
11 import matplotlib as mpl
12 import matplotlib.pyplot as plt
13 mpl.use('pgf')
14
15 pgf_with_latex = {
16     "pgf.texsystem": "pdflatex",
17     "pgf.preamble": "\n".join([
18         r"\usepackage[utf8x]{inputenc}",
19         r"\usepackage[T1]{fontenc}",
20         r"\usepackage{amsfonts}",
21         r"\usepackage{amsmath, amsthm, amssymb}",
22     ])
23 }
24 mpl.rcParams.update(pgf_with_latex)
25
26
27 def E(k, n):
28     """ Returns the energy of an electron with wavevector magnitude k,
29         E ~ k^n
30     """
31

```



```

32     return k**n
33
34 def DOS(Es):
35     """ Calculates the density of states given a vector of energy values.
36
37     Returns density of states g and center of the associated energy interval
38     .
39     """
40
41     # Use a histogram function to find the number energy states for each
42     # interval
43     g, edges = np.histogram(Es, bins=201)
44
45     # Calculate center of energy interval
46     centers = (edges[1:] + edges[0:-1])/2
47
48     return g, centers
49
50 # Define wavevector
51 ks = np.linspace(-1, 1, 501)
52
53 # Define wavevector matrices in all 3 directions
54 Kx, Ky, Kz = np.meshgrid(ks, ks, ks)
55
56 # Calculate matrix containing magnitude of wavevector
57 K = np.sqrt(Kx**2 + Ky**2 + Kz**2)
58
59 # Calculate matrix of energies
60 Es = E(K, 2)
61
62 # Use a histogram function to find the number energy states for each
63 # interval
64 g_3DEG, bin_centers = DOS(Es)
65
66 # Plot numerical result
67 fig, ax = plt.subplots(1, figsize=(3.4, 2.5))
68 ax.plot(bin_centers, g_3DEG/max(g_3DEG))
69
70 # Plot analytical result normalized based on numerical result
71 ax.plot(bin_centers, np.sqrt(bin_centers) \
72         * g_3DEG[2]/np.sqrt(bin_centers[2])/max(g_3DEG))
73
74 # Set line outside which DOS is not valid, since the k-vector is truncated
75 ax.plot(2*[E(ks[-1], 2)], [0, 1], 'k--')
76
77 ax.set_xlabel(r'$E/E_0$')
78 ax.set_ylabel(r'$g(E) \sim \text{[arb. units]}$')
79
80 plt.tight_layout()
81 plt.savefig('code7_1.pdf')
82
83 # We now do the same, but for different number of spatial dimensions and
84 # and power index n

```

```

81
82 # Define wavevector magnitude in different dimensions:
83 ks = np.linspace(-1, 1, 10001)
84 K1 = np.abs(ks)
85
86 ks = np.linspace(-1, 1, 2500)
87 k2 = np.meshgrid(ks, ks)
88 K2 = np.sqrt(k2[0]**2 + k2[1]**2)
89
90 ks = np.linspace(-1, 1, 500)
91 k3 = np.meshgrid(ks, ks, ks)
92 K3 = np.sqrt(k3[0]**2 + k3[1]**2 + k3[2]**2)
93
94 ns = [1, 2, 3, 4]
95
96 colors = ['C0', 'C1', 'C2', 'C4']
97
98 fig, ax = plt.subplots(1, 3, figsize=(6, 2.5))
99
100 for i, n in enumerate(ns):
101
102     Es = E(K1, n)
103     g, centers = DOS(Es)
104     ax[0].plot(centers, g/max(g), color=colors[i], label=n)
105
106
107     Es = E(K2, n)
108     g, centers = DOS(Es)
109     ax[1].plot(centers, g/max(g), color=colors[i])
110
111
112     Es = E(K3, n)
113     g, centers = DOS(Es)
114     ax[2].plot(centers, g/max(g), color=colors[i])
115
116
117 for d, ax_ in enumerate(ax, start=1):
118     ax_.set_xlim([0, E(1, 2)])
119     ax_.set_title(r'{}D'.format(d))
120     ax_.set_xlabel(r'$E/E_0$', labelpad=0)
121     ax_.set_xticks(np.linspace(0, 1, 5))
122     ax_.set_xticklabels([0.0, '', '', '', 1.0])
123     ax_.set_yticks(np.linspace(0, 1, 5))
124     ax_.set_yticklabels([])
125
126 ax[0].set_ylabel(r'$g(E)\text{~}\text{[arb. units]}$', labelpad=0)
127 ax[0].legend(frameon=False, title=r'$n$')
128 ax[0].set_yticklabels([0.0, '', '', '', 1.0])
129
130 plt.tight_layout()
131 plt.savefig('code7_2.pdf')
132

```

```

133
134 # Finally, we define the energy function for the tight binding model,
135 # and repeat the steps used above
136 def E_TB(kx, ky):
137     """2D Tight binding energy function."""
138
139     return - np.cos(kx) - np.cos(ky)
140
141
142 ks = np.linspace(-np.pi, np.pi, 2501)
143 k2 = np.meshgrid(ks, ks)
144 Es = E_TB(k2[0], k2[1])
145 g, centers = DOS(Es)
146
147 fig, ax = plt.subplots(1, figsize=(3.4, 2.5))
148 ax.plot(centers, g/max(g))
149 ax.set_xlabel(r'$E$')
150 ax.set_ylabel(r'$g(E)$~\text{[arb. units]}')
151
152 plt.tight_layout()
153 plt.savefig('code7_3.pdf')

```