Chapter 12
The Density of States

Many applications of quantum mechanics require the concept of density of states. The notion of density of states is not entirely unique. Depending on the context and the requirements of the problem at hand, it most often refers to the number of quantum states per volume and per unit of energy, or to the number of states in a volume unit $d^3\boldsymbol{k}$ in $\boldsymbol{k}$ space, and for both notions there are several variants of the density of states. Therefore the purpose of this chapter is not only to introduce the concept of density of states, but also to enumerate all the different definitions which are commonly used in physics.

Various forms of the density of states appear in numerous places in physics, e.g. in thermodynamics and optics we need the density of photon states in the derivation of Planck's law, in solid state physics the density of electron states appears in the integral of energy dependent functions over the Brillouin zone, in statistical physics we need it to calculate energy densities in physical systems, and in quantum mechanics we need it to calculate transition probabilities involving states in an energy continuum, e.g. to calculate electron emission probabilities for ionization or for the photoelectric effect, or to calculate scattering cross sections. Transition probabilities involving quantum states in an energy continuum (e.g. unbound states or states in an energy band in a solid) involve the density of states per particle as the number of states dn per unit of volume in $\boldsymbol{k}$ space,

$$dn = d^3\boldsymbol{k}. \tag{12.1}$$

More precisely, this is a density of states per spin or polarization or helicity states of a particle. Otherwise it would have to be multiplied by the number g of spin or helicity states.

The densities of electron states, photon states, and all kinds of quasiparticle states in materials are also very important quantities in materials science. These densities determine the momentum and energy distributions of (quasi)particles in materials, and the number of available states e.g. for charge or momentum transport,

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or for excitation of electrons or phonons. Densities of states therefore have profound impacts on electric and thermal conductivity and on optical properties of materials. We will see that there exist several ways to justify equation (12.1), and we will also explore the many different, but related definitions of the density of states.

12.1 Counting of oscillation modes

The basic notion of density of states concerns the $\boldsymbol{k}$ space density of linearly independent oscillation modes in a homogeneous volume. This is a very basic quantity in physics from which more advanced notions like local densities of states can be inferred. There are two basic ways to derive the $\boldsymbol{k}$ space density of states in a finite volume V. One of the derivations is more intuitive and the other one is slightly more formal, but the density of states is such an important concept that it is worthwhile to discuss both derivations.

The reasoning with periodic boundary conditions in a finite volume

The simplest derivation of (12.1) counts the number of independent oscillation modes in a rectangular cavity with periodic boundary conditions. A general wave vector can always be written in the form

$$\boldsymbol{k} = \frac{2\pi}{\lambda}\hat{\boldsymbol{k}} = \frac{2\pi}{\lambda}\sum_i \cos\theta_i\,\boldsymbol{e}_i,$$

where $\cos\theta_i$, $\sum_i \cos\theta_i^2 = 1$, are the directional cosines of the vector.

Suppose that the wave has to be periodic with periodicity L_i in direction $\boldsymbol{e}_i$. In that case the length L_i must be an integer multiple of the projection $\lambda_i = \lambda/\cos\theta_i$ of the wavelength onto the direction $\boldsymbol{e}_i$:

$$L_i = n_i\lambda_i = n_i\frac{\lambda}{\cos\theta_i}, \quad n_i \geq 0, \tag{12.2}$$

see Figure 12.1.

Equation (12.2) can be written in terms of the components of the wave vector $\boldsymbol{k}$,

$$k_i = \frac{2\pi}{\lambda}\cos\theta_i = \frac{2\pi}{\lambda_i} = 2\pi\frac{n_i}{L_i}.$$

The volume of a single state in $\boldsymbol{k}$-space is therefore (with g spin or helicity states per wave)

$$\left[\Delta^3\boldsymbol{k}\right]_{\text{single state}} = \frac{(2\pi)^3}{gV},$$

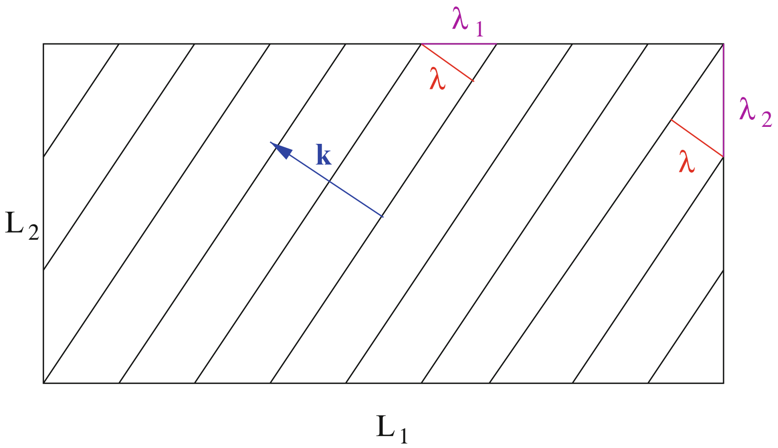

Fig. 12.1 A standing wave in a cavity with periodic boundary conditions

since g helicity states reside in a cell of volume $(2\pi)^3/V$ in $\boldsymbol{k}$-space. This yields the proportionality factor between the measure for the number of states dn and the volume measure in $\boldsymbol{k}$-space: The number dn of states in a volume $d^3\boldsymbol{k}$ in $\boldsymbol{k}$ space is

$$dn = d^3\boldsymbol{k} \Big/ \left[\Delta^3\boldsymbol{k}\right]_{\text{single state}} = \frac{gV}{8\pi^3} d^3\boldsymbol{k}. \tag{12.3}$$

Inclusion of the factor g corresponds to a summation over all possible polarizations or helicities. This version of the density of states is often employed in thermodynamics and statistical physics. In quantum mechanics and scattering theory we often need the density of states with a given polarization or helicity,

$$dn = \frac{V}{8\pi^3} d^3\boldsymbol{k}. \tag{12.4}$$

The quantity $dn/d^3\boldsymbol{k} = V/(2\pi)^3$ is the density of polarized states (if the system can have polarization) in $\boldsymbol{k}$ space, and $dn/(Vd^3\boldsymbol{k}) = 1/(2\pi)^3$ is the corresponding density of states in phase space. We will mostly use the density (12.4) or its continuum limit, i.e. we will usually count states with a given polarization or helicity, e.g. states of spin up electrons, states of photons of given polarization, etc.

The reasoning based on the completeness of plane wave states

A slightly more formal reasoning is based on the completeness of Fourier monomials. The Fourier monomials

$$\langle \boldsymbol{x}|\boldsymbol{n}\rangle = \frac{1}{\sqrt{V}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}) = \frac{1}{\sqrt{V}} \exp\left(2\pi\mathrm{i}\sum_i \frac{n_i x_i}{L_i}\right) \tag{12.5}$$

provide a complete set of functions in a box of lengths L_i, cf. (10.2) and (10.3) for the one-dimensional versions of the following equations:

$$\frac{1}{V}\int_V d^3\boldsymbol{x}\,\exp\left(2\pi\mathrm{i}\sum_i \frac{n_i-n_i'}{L_i}x_i\right)=\delta_{\boldsymbol{n},\boldsymbol{n}'},$$

$$\frac{1}{V}\sum_{\boldsymbol{n}}\exp\left(2\pi\mathrm{i}\sum_i n_i\frac{x_i-x_i'}{L_i}\right)=\delta(\boldsymbol{x}-\boldsymbol{x}').$$

Therefore we find again $k_i = 2\pi n_i/L_i$ for the components of the $\boldsymbol{k}$ vectors, and the volume per base oscillation mode (with fixed polarization) is again

$$\Delta^3\boldsymbol{k}\Big|_{\text{single mode}}=\frac{8\pi^3}{V}.$$

This yields again the equation (12.4),

$$dn=\frac{V}{8\pi^3}d^3\boldsymbol{k}.$$

We remark that the measure dn for the number of states in $\boldsymbol{k}$-space (12.4) can also be written in terms of the wave numbers $\tilde{\nu}_i \equiv 1/\lambda_i = k_i/2\pi$,

$$dn=\frac{V}{8\pi^3}d^3\boldsymbol{k}=Vd^3\tilde{\boldsymbol{\nu}}=Vd^3\frac{1}{\boldsymbol{\lambda}}.$$

If we also replace the volume V in position space with the volume measure $d^3\boldsymbol{x}$, we find a particularly intuitive and suggestive form for the corresponding measure of states in phase space,

$$dn=d^3\boldsymbol{x}\,d^3\tilde{\boldsymbol{\nu}}=d^3\boldsymbol{x}\,d^3\frac{1}{\boldsymbol{\lambda}}=\frac{d^3\boldsymbol{x}\,d^3\boldsymbol{p}}{h^3}.$$

Here $\boldsymbol{\lambda}=\lambda\hat{\boldsymbol{k}}$, and we define the "inverse" vector as $1/\boldsymbol{\lambda}\equiv\boldsymbol{\lambda}/\lambda^2$.

12.2 The continuum limit

In the limit $V\to\infty$, the discrete enumerable set of normalized plane waves in a cubic volume V, $\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})/\sqrt{V}$, $\boldsymbol{k}=2\pi\boldsymbol{n}/L=2\pi\boldsymbol{n}/V^{1/3}$, is replaced by the continuous non-enumerable set $\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})/\sqrt{2\pi}^3$. We have derived the completeness relation for the continuous Fourier monomials in Section 2.1, see equations (2.2) and (2.9). However, for the discussion of the continuum limit of (12.4) it is useful to revisit the completeness relation of the continuous Fourier monomials as a continuum limit of the completeness relation of Fourier monomials in finite volume.

We are using $\Delta^3\boldsymbol{n} = 1$ for the volume of a triplet of integers in $\mathbb{Z}^3$. The completeness relation for the Fourier monomials in a cubic box can then be written as

$$\begin{aligned}
\delta(\boldsymbol{x}-\boldsymbol{x}') &= \frac{1}{V}\sum_{\boldsymbol{n}}\exp\!\left(\frac{2\pi\mathrm{i}}{V^{1/3}}\boldsymbol{n}\cdot(\boldsymbol{x}-\boldsymbol{x}')\right)\\
&= \frac{1}{V}\sum_{\boldsymbol{n}}\Delta^3\boldsymbol{n}\,\exp\!\left(\frac{2\pi\mathrm{i}}{V^{1/3}}\boldsymbol{n}\cdot(\boldsymbol{x}-\boldsymbol{x}')\right)\\
&= \frac{1}{V}\sum_{\boldsymbol{k}}\frac{V}{(2\pi)^3}\Delta^3\boldsymbol{k}\,\exp\!\big[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')\big]\\
&\to \frac{1}{(2\pi)^3}\int d^3\boldsymbol{k}\,\exp\!\big[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')\big],
\end{aligned} \tag{12.6}$$

where we have used the fact that the volume cancels to take the continuum limit in the final step.

This corresponds to the substitution $V \Rightarrow (2\pi)^3$ in the plane waves, and the corresponding substitution for the measure for the number of states is indeed

$$dn = \frac{V}{(2\pi)^3}d^3\boldsymbol{k} \;\;\Rightarrow\;\; d^3\boldsymbol{k}. \tag{12.7}$$

Note that either way, the density of states per volume V of a particle with fixed helicity or spin is

$$\frac{dn}{V} = \frac{d^3\boldsymbol{k}}{(2\pi)^3}, \tag{12.8}$$

irrespective of whether we have taken the continuum limit or not. However, please also note that in the continuum limit both the differential number of states $dn = d^3\boldsymbol{k}$ and the number of states per volume $dn/V = d^3\boldsymbol{k}/(2\pi)^3$ come with dimensions length^{-3}.

The "dimensionally wrong" density of states $dn/d^3\boldsymbol{k} = 1$ in $\boldsymbol{k}$ space is a consequence of the cancellation of V in (12.6) and the ensuing interpretation of $\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})/\sqrt{2\pi}^3$ as the properly normalized plane wave states in the continuum limit. This has shifted the length dimension from the states

$$\dim\!\Big[\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})/\sqrt{V}\Big] = \ell^{-3/2} \to \dim\!\Big[\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})/\sqrt{2\pi}^3\Big] = 1$$

into the $\boldsymbol{k}$ space measure of states,

$$\dim\bigl[dn = d^3\boldsymbol{k}V/(2\pi)^3\bigr] = 1 \to \dim\bigl[dn = d^3\boldsymbol{k}\bigr] = \ell^{-3}.$$

We have to keep this in mind when we are using dimensional analysis of quantum mechanical transition amplitudes in time-dependent perturbation theory in Chapters 13 and 18.

Another reasoning for the continuum limit

We consider the matrix element of the time evolution operator $U_D(t,t')$ between a bound hydrogen state $|n,\ell,m_\ell\rangle$ and a plane wave $|\boldsymbol{k}\rangle$. The definition of U_D and the motivation for considering its matrix elements will be given in the following chapter. For now we only need to know that it is a unitary operator which describes e.g. how bound hydrogen eigenstates are scattered into other states under a time-dependent perturbation of the hydrogen atom.

Unitarity of $U_D(t,t')$ and the completeness relation for plane waves imply

$$\int d^3\boldsymbol{k}\left|\langle\boldsymbol{k}|U_D(t,t')|n,\ell,m_\ell\rangle\right|^2 = 1.$$

This tells us that we can interprete $|\langle\boldsymbol{k}|U_D(t,t')|n,\ell,m_\ell\rangle|^2$ as a probability density for the system to end up in a plane wave state $|\boldsymbol{k}\rangle$, and $d^3\boldsymbol{k}$ as a measure for the number of states, such that the probability for the system to end up in a region $\mathcal{K}$ in $\boldsymbol{k}$ space is

$$P_{n,\ell,m_\ell\to\mathcal{K}}(t,t') = \int_{\mathcal{K}} d^3\boldsymbol{k}\left|\langle\boldsymbol{k}|U_D(t,t')|n,\ell,m_\ell\rangle\right|^2.$$

This confirms yet again that $dn = d^3\boldsymbol{k}$ is the correct density of states in $\boldsymbol{k}$ space in the continuum limit.

Different forms of the density of states in a homogeneous medium

We may or may not include the number g of helicity or spin states in the density of states, we can normalize to finite volume V or take the continuum limit $V \to \infty$, and we may also use the number of states per $\boldsymbol{k}$ space volume and per direct volume V (i.e. calculate the density of states in phase space). All these simple alternatives amount to eight basic options for the density of states in $\boldsymbol{k}$ space,

$$dn = [g]\left[\frac{[V]}{8\pi^3}\right]d^3\boldsymbol{k}.$$

The first term in square brackets is included if we sum over all possible polarizations of the particle, and the fraction $V/(8\pi^3)$ is included if we use box normalization. The volume factor is not included if the density of states is also counted per volume in position space, dn/V. The fraction $V/(8\pi^3)$ in dn disappears in the continuum limit.

12.3 The density of states in the energy scale

In solid state physics (and in variants of time-dependent perturbation theory and scattering theory) one is often interested in transforming $d^3\boldsymbol{k}$ to variables $d^2\boldsymbol{k}_\parallel$ parallel to surfaces of constant energy $E(\boldsymbol{k})$ in $\boldsymbol{k}$ space and the energy E, which increases orthogonal to the surfaces of constant energy. The normalized unit vector in the direction of increasing E is

$$\hat{\boldsymbol{k}}_\perp = \frac{\partial E(\boldsymbol{k})/\partial \boldsymbol{k}}{|\partial E(\boldsymbol{k})/\partial \boldsymbol{k}|} = \frac{\boldsymbol{v}(\boldsymbol{k})}{|\boldsymbol{v}(\boldsymbol{k})|}$$

(recall that $\boldsymbol{v}(\boldsymbol{k}) = \hbar^{-1}\partial E(\boldsymbol{k})/\partial \boldsymbol{k}$ is the group velocity). Therefore we have

$$dk_\perp = d\boldsymbol{k}\cdot\hat{\boldsymbol{k}}_\perp = \frac{d\boldsymbol{k}\cdot\partial E(\boldsymbol{k})/\partial \boldsymbol{k}}{|\partial E(\boldsymbol{k})/\partial \boldsymbol{k}|} = \frac{dE}{|\partial E(\boldsymbol{k})/\partial \boldsymbol{k}|} = \frac{dE}{\hbar|\boldsymbol{v}(\boldsymbol{k})|}$$

and

$$d^3\boldsymbol{k} = d^2\boldsymbol{k}_\parallel \frac{dE}{|\partial E(\boldsymbol{k})/\partial \boldsymbol{k}|}.$$

Here $d^2\boldsymbol{k}_\parallel$ is some appropriate measure for coordinates along the constant energy surfaces.

An isotropic dispersion relation, $E(\boldsymbol{k}) = E(k)$, yields

$$d^3\boldsymbol{k} = d^2\Omega_k k^2 \frac{dE}{dE/dk}.$$

The corresponding number of states is then

$$dn = [g]\left[\frac{[V]}{8\pi^3}\right] d^2\Omega_k k^2 \frac{dE}{|dE/dk|} = \varrho(E)dEd^2\Omega_k, \tag{12.9}$$

with a density of states *per energy* or density of states *in the energy scale*

$$\varrho(E) = [g]\left[\frac{[V]}{8\pi^3}\right]\frac{k^2}{|dE/dk|}. \tag{12.10}$$

Here the absolute value $|dE/dk|$ is taken in the denominator, because in cases where $dE/dk < 0$, the convention is to substitute an integral in positive dk direction with an integral in positive dE direction in the summation over states,

$$dk = \frac{dE}{dE/dk} \to \frac{dE}{|dE/dk|}.$$

In isotropic problems the angular variables are often integrated over, and one uses the convention

$$dn \to \varrho(E)dE$$

with the factor 4π included in ϱ. Altogether this leaves us with the following sixteen possibilities for the density of states in the energy scale,

$$\varrho(E) = [g]\left[\frac{[V]}{8\pi^3}\right][4\pi]\,\frac{k^2}{|dE/dk|}. \tag{12.11}$$

We remark that generalization of the previous arguments to d spatial dimensions yields the following results for the density of states,

$$dn = [g]\left[\frac{[V]}{(2\pi)^d}\right]d^d\boldsymbol{k}, \quad \varrho_d(E) = [g]\left[\frac{[V]}{(2\pi)^d}\right]\left[\frac{2\sqrt{\pi}^d}{\Gamma(d/2)}\right]\frac{k^{d-1}}{|dE/dk|}, \tag{12.12}$$

where $S_{d-1} = 2\sqrt{\pi}^d/\Gamma(d/2)$ is the $(d-1)$-dimensional hyper-area of a unit sphere in d dimensions.

12.4 Density of states for free non-relativistic particles and for radiation

The free non-relativistic particle satisfies $E = \hbar^2k^2/2m$, and equation (12.12) yields the following forms of the density of states in the energy scale in d dimensions,

$$\varrho_d(E) = \Theta(E)\,[g]\left[\frac{[V]}{(2\pi)^d}\right]\left[\frac{2\sqrt{\pi}^d}{\Gamma(d/2)}\right]\left(\frac{\sqrt{m}}{\hbar}\right)^d\sqrt{2E}^{d-2}.$$

The most commonly used version gives the density of free non-relativistic states per volume and per energy in d dimensions as

$$\varrho_d(E) = g\Theta(E)\sqrt{\frac{m}{2\pi}}^d\,\frac{\sqrt{E}^{d-2}}{\Gamma(d/2)\hbar^d}. \tag{12.13}$$

For $d = 3$ this yields the density of states in a free electron model for metals. For other materials this equation can be used to calculate the density of electron states near the minimum of an energy band or the density of hole states near the maximum of an energy band if we replace E with the difference to the local minimum or maximum in energy: $E \to E - E_{min}$ or $E \to E_{max} - E$. In these cases m is the effective electron or hole mass near E_{min} or E_{max}, respectively. Equation (12.13) is also often employed for $d = 1$ and $d = 2$ to estimate the density of states in quantum wires or quantum wells.

The energy of a photon of frequency f is $E = hf = \hbar ck$ and we have $g = 2$ independent polarization states. Equations (12.3) or (12.11) therefore yield the following expressions for the density of photon states per volume and per unit of energy,

$$\varrho(E) = \frac{dn}{VdE} = \frac{2}{8\pi^3} 4\pi k^2 \frac{dk}{dE} = \frac{E^2}{\pi^2(\hbar c)^3},$$

or in d dimensions (with $g = d - 1$ polarizations),

$$\varrho_d(E) = \frac{(d-1)E^{d-1}}{2^{d-1}\pi^{d/2}\Gamma(d/2)(\hbar c)^d}.$$

The density of photon states (per volume V) in the frequency scale follows as

$$\varrho_d(f) = \frac{dn}{Vdf} = \frac{2(d-1)\pi^{d/2}}{\Gamma(d/2)} \frac{f^{d-1}}{c^d}.$$

For $d = 3$ this is equation (1.6) which we have used in the derivation of Planck's law.

12.5 The density of states for other quantum systems

It is also useful to note that we can express the density of states per volume in plane waves trivially through the corresponding wave functions,

$$\frac{dn}{V} = \frac{d^3\boldsymbol{k}}{(2\pi)^3} = d^3\boldsymbol{k}\, |\langle \boldsymbol{x}|\boldsymbol{k}\rangle|^2 .$$

This suggests the following identification of the number of states per volume in terms of quantum states which are labeled through a set of quantum numbers α,

$$\frac{dn}{V}(\boldsymbol{x}) = d\alpha\, |\langle \boldsymbol{x}|\alpha\rangle|^2 . \tag{12.14}$$

From this observation we can infer a generalization of the density of states per volume and per unit of energy which also holds for discrete spectra. Suppose the Hamiltonian H has a discrete spectrum E_n and continuous spectra in ranges $E_{b1} \leq E \leq E_{b2}$. We use $\alpha = (E, \nu)$ for the set of quantum numbers, where ν is a set of degeneracy indices. Then the previous identification yields the density of states per volume and per energy as

$$\begin{aligned}\varrho(E,\boldsymbol{x}) = \sum_n \delta(E-E_n) \sum\!\!\!\!\!\!\int d\nu_n \, |\langle \boldsymbol{x}|E_n, \nu_n\rangle|^2 \\ + \sum_b \Theta(E-E_{b1})\Theta(E_{b2}-E) \sum\!\!\!\!\!\!\int d\nu(E) \, |\langle \boldsymbol{x}|E, \nu(E)\rangle|^2 . \quad (12.15)\end{aligned}$$

E.g. the density of states per volume and per energy for the hydrogen atom would be (with factors of 2 from summation over spins)

$$\begin{aligned}\varrho(E,\boldsymbol{x}) = 2\sum_{n=1}^{\infty} \delta(E-E_n) \sum_{\ell=0}^{n-1} \sum_{m_\ell=-\ell}^{\ell} |\langle \boldsymbol{x}|n,\ell,m_\ell\rangle|^2 \\ + \Theta(E) \sum_{\ell=0}^{\infty} \sum_{m_\ell=-\ell}^{\ell} \frac{1}{\hbar^3}\sqrt{(2m)^3E}\, |\langle \boldsymbol{x}|k,\ell,m_\ell\rangle|^2 , \quad (12.16)\end{aligned}$$

where $\langle \boldsymbol{x}|k,\ell,m_\ell\rangle$ are the Coulomb waves $\psi_{k,\ell,m_\ell}(\boldsymbol{x})$ from Section 7.9 and $\sqrt{(2m)^3E}/\hbar^3 = 2k^2dk/dE$.

A short hand version of equation (12.15) is

$$\varrho(E,\boldsymbol{x}) = \sum\!\!\!\!\!\!\int dE' \, d\nu(E') \, \delta(E-E') \left|\langle \boldsymbol{x}|E', \nu(E')\rangle\right|^2 . \quad (12.17)$$

Note that for each quantum system, the total number of single-particle states per volume diverges in a very specific way,

$$\int \frac{dn}{V} = g\langle \boldsymbol{x}|\boldsymbol{x}\rangle = g\delta(\mathbf{0}).$$

12.6 Problems

12.1. We consider a free gas of spin 1/2 fermions in a finite volume $V = L^3$ with periodic boundary conditions. This implies the constraints

$$k_i = \frac{2\pi}{L}n_i, \quad n_i \in \mathbb{Z}$$

on the components of the wave vector.

Our fermion gas contains $N \gg 1$ particles, and we assume it to be in the state of minimal energy. How large is the maximal momentum $p_F = \hbar k_F$ (the *Fermi momentum*) in the fermi gas?

You have to take into account that only two fermions can have the same momentum.

Solution. With $N \gg 1$ we have $\lambda_F \ll L$ or $k_F \gg \frac{2\pi}{L}$. The number of states with momenta $p \leq p_F$ is then

$$2\frac{4\pi}{3}k_F^3\frac{L^3}{8\pi^3} = \frac{1}{3\pi^2}k_F^3 L^3 = N,$$

and therefore

$$k_F = \frac{1}{L}\left(3\pi^2 N\right)^{\frac{1}{3}} = \left(3\pi^2 n\right)^{\frac{1}{3}}, \quad p_F = \hbar k_F, \tag{12.18}$$

where $n = N/V$ is the particle density.

12.2. The equation (12.12) for the density of states in d dimensions holds for isotropic dispersion relations $E = E(|\boldsymbol{k}|)$. We used $k \equiv |\boldsymbol{k}|$ in (12.12).

For one-dimensional models that equation yields the density of states in the energy scale per volume $V \equiv a$ (a lattice constant) and per helicity state as

$$\varrho_1(E) = \frac{1}{ag}\frac{dn}{dE} = \frac{1}{2\pi} \times 2 \times \left|\frac{d|k|}{dE}\right|. \tag{12.19}$$

The factor of 2 comes from the "volume" $S_0 = [2\sqrt{\pi}^d/\Gamma(d/2)]_{d=1}$ of the zero-dimensional unit sphere. This sphere consists of the two points 1 and -1. Is equation (12.19) correct? Or should we abandon the factor of 2?

12.3. Equation (12.14) for the local density of states yields for one-dimensional lattices with volume $V = a$ and Bloch states (10.8) the local density of states in the k scale as

$$\varrho(k,x) = \frac{dn}{agdk}(x) = \sum_n |\psi_n(k,x)|^2.$$

Note that we also divided out the number g of spin or helicity states, which is included as a discrete parameter in the set of quantum numbers α in (12.14).

Show that transformation to the energy scale and spatial averaging reproduces the isotropic result (12.19),

$$\varrho(E) = \frac{1}{a}\int_0^a dx\, \varrho(E,x) = \frac{1}{\pi}\left|\frac{d|k|}{dE}\right|.$$

12.4. We consider the Kronig-Penney model from Section 10.4.

Show for $E > 0$ that the spatially averaged one-dimensional density of states in the energy scale,

$$\varrho(E) = \frac{dn}{agdE} = \frac{1}{\pi}\left|\frac{d|k|}{dE}\right|,$$

is given by

$$\varrho(E) = \frac{m}{\pi\hbar^2 K}\left|\left(1+\frac{u}{(Ka)^2}\right)\sin(Ka) - \frac{u}{Ka}\cos(Ka)\right| \times\left[\left(1-\frac{u^2}{(Ka)^2}\right)\sin^2(Ka) - \frac{u}{Ka}\sin(2Ka)\right]^{-1/2}, \qquad (12.20)$$

with $K = \sqrt{2mE}/\hbar$. This equation only applies where states exist, i.e. where the condition (10.35) is met.

The resulting density of states for $u = 5$ in the region of the first two energy bands is plotted in Figure 12.2 for a lattice constant $a = 3.5$ Å.

12.5. Calculate the density of states in the energy scale for free unpolarized electrons in three dimensions if you *cannot* assume that the kinetic energy of the electrons is much smaller than their rest energy.

Which result do you get in the non-relativistic limit?

Derive the corresponding results also in d spatial dimensions.

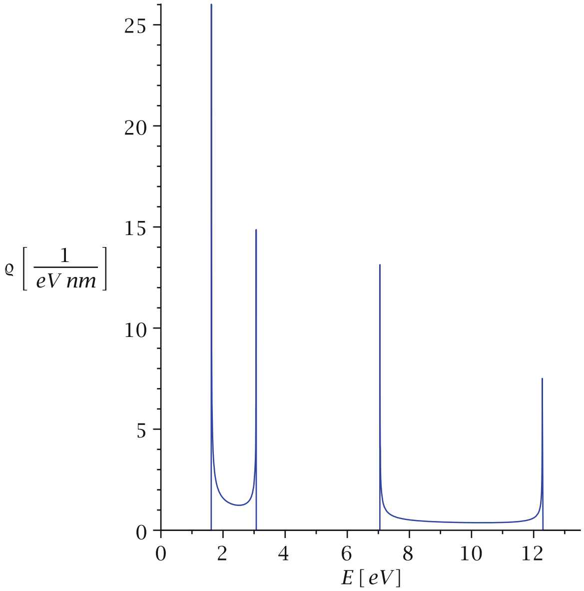

Fig. 12.2 The one-dimensional density of states in the energy scale (12.20) for $u = 5$ and a lattice constant $a = 3.5$ Å. The energy scale covers the first two energy bands $E_0(k)$ and $E_1(k)$, cf. Figure 10.2

Result. The relativistic dispersion relation $E = \hbar c\sqrt{k^2 + (mc/\hbar)^2}$ yields for particles with g helicity (or spin or polarization) states the density of states per volume and in the energy scale

$$\begin{aligned}\varrho(E) &= \frac{dn}{dVdE} = \frac{g}{(2\pi)^d}\frac{2\sqrt{\pi}^d}{\Gamma(d/2)}k^{d-1}\frac{dk}{dE} \\ &= \frac{2g\Theta(E - mc^2)}{(2\sqrt{\pi}\hbar c)^d\Gamma(d/2)}E\sqrt{E^2 - m^2c^4}^{d-2}.\end{aligned} \tag{12.21}$$

For the comparison with the non-relativistic limit we should write this in terms of the kinetic energy $K = E - mc^2$, because K is usually denoted as the energy of the particle in the non-relativistic limit,

$$\varrho(K) = \frac{2g\Theta(K)}{(2\sqrt{\pi}\hbar c)^d\Gamma(d/2)}(K + mc^2)\sqrt{K(K + 2mc^2)}^{d-2}. \tag{12.22}$$

This yields the non-relativistic result (12.13) (with the substitution $E_{non-rel.} = K$) in the limit $K \ll mc^2$.

Note that use of $E = \pm\hbar c\sqrt{k^2 + (mc/\hbar)^2}$ yields a symmetric density of states which includes the anti-particles as negative energy states,

$$\hat{\varrho}(E) = \varrho(E) + \overline{\varrho}(\overline{E}) = \frac{2g\Theta(E^2 - m^2c^4)}{(2\sqrt{\pi}\hbar c)^d\Gamma(d/2)}|E|\sqrt{E^2 - m^2c^4}^{d-2}. \tag{12.23}$$

Here $\overline{E} = -E > mc^2$ corresponds to the energy of the anti-particles. As for the factor g, we just remark for completeness that a massive vector field in $d + 1$ space-time dimensions has $g_d = d$ possible polarizations. Furthermore, a spinor in $d + 1$ space-time dimensions has $2^{\lfloor(d+1)/2\rfloor}$ components which describe both particles and anti-particles, and therefore an electron in $d + 1$ space-time dimensions has $g_d = 2^{\lfloor(d-1)/2\rfloor}$ spin components. The floor function used here yields $\lfloor n/2\rfloor = n/2$ if n is even, $\lfloor n/2\rfloor = (n - 1)/2$ if n is odd. Please see Chapter 21 and Appendix G (note that d denotes the number of space-time dimensions in Appendix G).