Problem set: Electronic Density of States

Consider the general definition of $d$-dimensional density of states (DOS) for one band $E(k)$

\[ g(E_0) = \frac{1}{N} \sum_{k} \delta(E - E(k)) = \frac{2}{N} \sum_{k} \delta(E - E(k)) = \frac{2V}{N} \int_{BZ} \frac{d^{d}k}{(2\pi)^{d}} \delta(E_0 - E(k)) = \frac{2V}{N} \int_{S(E_0)} \frac{dS}{(2\pi)^{d}} \frac{1}{|\partial E(k)/\partial k|} \]  

where the prefactor two indicates the spin-degeneracy and $S(E_0)$ is the isosurface the reciprocal space defined by $E(k) = E_0$.

7.1. Electrons in the continuum

Calculate the DOS for different analytically-known energy dispersions.

(a) Massive and massless free particles in $d$ dimensions

Calculate the density of states $g(E)$ for massless and massive particles in $d = 1$, 2 and 3 dimensions, and prove the the following results.

<table>
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<tr>
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<th>$d = 1$</th>
<th>$d = 2$</th>
<th>$d = 3$</th>
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</thead>
<tbody>
<tr>
<td>massless $(E \sim k)$</td>
<td>$g(E) = \text{const}$</td>
<td>$g(E) \sim E$</td>
<td>$g(E) \sim E^2$</td>
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<tr>
<td>massive $(E \sim k^2)$</td>
<td>$g(E) \sim 1/\sqrt{E}$</td>
<td>$g(E) = \text{const}$</td>
<td>$g(E) \sim \sqrt{E}$</td>
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(b) DOS in superconductors

In the BCS-theory of superconductivity\(^1\) the excitation spectrum of single-electron states is given by:

\[ E(k) = E_F + \text{sign}(\varepsilon(k) - E_F) \sqrt{(\varepsilon(k) - E_F)^2 + \Delta(k)^2} \]

where $\varepsilon(k)$ is the electron energy in absence of superconductivity and $E_F$ is the Fermi energy. A simplified interaction leads to constant $\Delta(k) = \Delta$. Starting from the DOS of the system without superconductance $g(\varepsilon)$, calculate the DOS of the full system $g'(E)$, assuming that $E_F$ is not close to a band-edge.

Hint: Consider the integral-definition of the DOS: For constant $\Delta$, the problem boils down to a change of variables...

(c) **Hybridized states**

If electrons can jump between a broad band (described by $E_c(k)$) and a narrow energy level at $E_0$, then the band structure exhibits signs of hybridization: A mixing of electronic states when the $E_c(k)$ and the $E_0$ energies are close. In a simple model, the hybridized energy levels can be calculated as

$$E'(k) = \frac{(E_c(k) + E_0)}{2} \pm \sqrt{\frac{(E_c(k) - E_0)^2}{4} + \Delta^2}$$

where $\Delta$ is the coupling parameter, proportional to the probability of hopping events per time.

Assume that the broad band has the constant DOS $g_c(E) = g_0$ for $E_1 < E < E_2$ (with the bandwidth $W = E_2 - E_1$) and $g_c(E) = 0$ otherwise. The DOS of the narrow band is sharply peaked with the same total number of states: $g = g_0 W \delta(E - E_0)$. Calculate the DOS for the hybridized system.

(d) **Two dimensional electron gas (2DEG)**

The dimensionality of a real electron system can be reduced by confining potentials in certain directions. Consider an electron gas in the potential

$$V(x, y, z) = V_0 \Theta(|z| - \ell/2).$$

- Plot the DOS in the limit $V_0 \to \infty$?
- Assume $\ell = 10$ nm. Up to which temperature $T$ can we consider the electrons to be two-dimensional?
- If we can produce a potential with $V_0 = 100$ meV and reach $T = 20$ mK, for which range of thicknesses $\ell$ can we consider the system a 2DEG?
7.2. Tight binding electrons

The energy band of an anisotropic orthorhombic lattice in the s-orbital tight-binding approximation leads to the following dispersion relation

\[ E(\mathbf{k}) = -\frac{E_0}{2} \left[ A_x \cos (k_x a_x) + A_y \cos (k_y a_y) + A_z \cos (k_z a_z) \right], \]

\((E_0 = 1 \text{ eV} \text{ defines the energy scale}).\) We want to investigate the crossover between \(d = 1\) and \(d = 3\) electron systems, so we assume \(A_x = 1, A_y = A_z = B \in [0, 1].\)

The figure below shows the DOS calculated numerically for different values of \(B\) by statistical integration of Eq. (1).

(a) Consider \(B \ll 1\): What is the shape of the energy isolines cuts in the \(k_x-k_y\)-plane?

(b) Show that for a half-filled band the DOS (and therefore thermodynamic properties like total energy, total number of electrons and specific heat) of this system are similar to a truly one-dimensional electron gas.

\textbf{Hint:} A simple approximation of the isolines at \(E = 0\) allows direct integration.

(c) For low electron densities, the system differs considerably from a truly 1D system even at low \(B\). Estimate the electron density, at which the crossover happens.

(d) Compare the behavior at the band edge between \(d = 1\) and \(d = 3\) system.
(e) Consider now the case $A_x = 0$ and $A_y = A_z = 1$ as shown below and explain the behavior of the DOS around $E = 0$!

![Graph showing DOS for $A_x = 0, A_y = A_z = 1$]

7.3. Infinite dimensional DOS (optional)

The figure below shows the DOS for an isotropic tight-binding lattice in $d = 1, 2, 3, 4$ dimensions. The bandwidth is set to $\sqrt{a}$. What is the DOS for $d \to \infty$? Why has the bandwidth to be scaled like $\sqrt{d}$? What is its physical meaning?

![Graphs showing DOS for different $d$ values]

Hint: Consider calculating the problem via Monte Carlo integration: The integration variables $k = (k_1, k_2, ..., k_d)$ are turned into independent uniformly distributed random variables in the interval $[0, 2\pi/a]$. The DOS $g(k)$ is the distribution of the sum $E(k) = \frac{E_0}{2\sqrt{d}} \sum_{i=1}^{d} (-\cos k_i a)$ which, for $d \to \infty$, follows the central limit theorem.

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