University of Regensburg Summer Semester 2008

Quantum Theory of Condensed Matter

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Sheet 13

1. Density of states of an infinite ribbon (analytics)

Let's us consider an infinite ribbon made of N_y chains of atoms organized in a square lattice (see Fig. 1). The valence (spinless) electrons are described by the tight binding Hamiltonian:

$$H = \lim_{N_x \to \infty} t \sum_{\langle i,j \rangle} c_i^\dagger c_j$$

where the sum runs over nearest neighbors and we assume periodic boundary conditions in the x direction (*i.e.* $N_x + 1 = 1$).

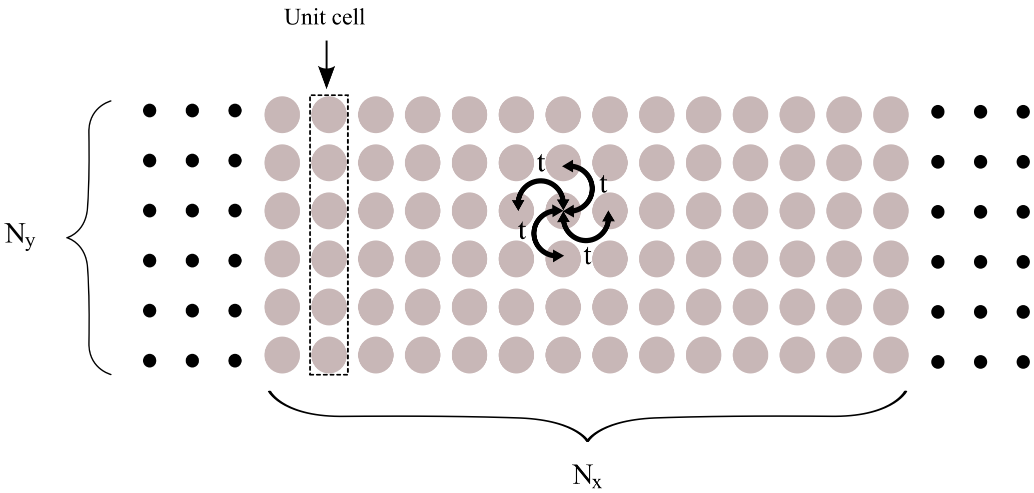

Fig. 1

1. The ribbon is invariant under translation in the x direction by any multiple of lattice unit. Use the Bloch theorem to diagonalize the Hamiltonian for the infinite system and calculate the band structure for the ribbon for the case with $N_y = 2, 3$. How many bands do you obtain in each case?

2. Prove that the ribbon is equivalent to $2 \times N_y$ independent chains of atoms with on-site energies equal to the eigenenergies of the isolated unit cell and the same hopping parameter t of the ribbon.

3. Prove that the density of states (normalized to the length) of the ribbon reads:

$$\tilde{\rho}(E) \equiv \lim_{N_x \to \infty} \frac{1}{N_x} \sum_\alpha \delta(E - \epsilon_\alpha) = \sum_{i=1}^{N_y} \frac{1}{\pi \sqrt{4t^2 - (E - \epsilon_i)^2}}$$

   where α is a collection of quantum numbers labeling the eigenstates of the ribbon and ϵ_i are the eigenenergies of the isolated unit cell.

2. Density of states of an infinite ribbon (numerics)

The density of states of a system can be calculated with the help of the Green's functions using the formula:

$$\rho(E) = \frac{1}{2\pi}\mathrm{Tr}\{-2\mathrm{Im}[G^r(E)]\}$$

where $G^r(E)$ is the retarded Green's function for the system defined as $G^r(E) = (E - H + i\eta)^{-1}$.

1. Construct numerically the Hamiltonian for a finite size ribbon with $N_y = 2, 3$ and $N_x = 2, 20, 200$ and using the definition given above calculate the corresponding Green's function. *Hint:* Values of η in the order of $\frac{4t}{N_x}$ are a good compromise between the requirement of small η and the energy grid necessary to resolve the structure of the Green's function.

2. Starting from the Green's function calculated at the previous point, calculate the density of states normalized to the ribbon length $\tilde{\rho}(E) \equiv \frac{\rho(E)}{N_x}$ and compare the result with the analytical one obtained at the previous point. *Hint:* Remember that the trace of a matrix is invariant under change of basis. The efficiency of the numerical calculation is in this case enormously enhanced in the eigenstate basis.

3. If you have difficulties with the numerical part of the sheet you can start by following the suggested Matlab solution that you find in the next pages. You can also download the code from the web:

   `http://homepages-nw.uni-r.de/~doa17296/fisica/fisica.html`

Frohes Schaffen!

```
clear all
                              %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
                              %                                  %
                              %     The 1D stripe and tube       %
                              %                                  %
                              %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
                              %                                  %
                              %   Solution to Sheet13 of QTKM1   %
                              %                                  %
                              %               SS08               %
                              %                                  %
                              %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

E_0 = 0;%----------------------- On-site energy for the electrons in the ribbon
b_intra = -1;%------------------ Hopping parameter between sites in the same unit cell
b_inter = 1*b_intra;%----------- Hopping parameters between NN_atoms in different cells
per = 0;%----------------------- Parameter for the boudary conditions per unit cell:
                               % 1 periodic: we are dealing with an infinite tube;
                               % 0 Dirichlet: we are dealing with a ribbon.
N_x= 100;%------------------------ Number of unit cells
N_y=4;%------------------------ Number of atoms per unit cell
eta = abs(b_inter)/20;%--------------------- Infinitesimal broadening

Emin = 2.5*(b_intra+b_inter);%-- Inferior limit of interesting energies
Evet = Emin:eta/5:-Emin;%Energy range of calculaation


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 1) Construction of the Hamiltonian for the unit cell
H_0 = E_0*diag(ones(1,N_y)) + b_intra*(diag(ones(1,N_y-1),1) + diag(ones(1,N_y-1),-1));

% Implementation of the ribbon/tube boundary conditions
% A ribbon of lateral dimension 2 is also a tube!!!
if N_y > 2
H_0(1,N_y) = per*b_intra;
H_0(N_y,1) = per*b_intra;
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 2) Construction of the tunnelling Hamiltonian between unit cells
T_0 = b_inter*diag(ones(1,N_y),0);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 3) Recursive construction of the total Haniltonian. H for N unit cells is
% contructed from H for N-1 unit cells
H = H_0;
for extra = 1:N_x-1
H_new = [H, [zeros(N_y*(extra-1),N_y);T_0]; [zeros(N_y*(extra-1),N_y);T_0]',H_0];
H = H_new;
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 4) Implementation of the periodic boundary conditions at the border of
% the finite ribbon
if N_x > 2
H(N_y*(N_x-1) + 1:N_y*N_x,1:N_y) = T_0;
H(1:N_y,N_y*(N_x-1) + 1:N_y*N_x) = T_0';
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 5) Diagonalization of the Hamiltonian
E_a = eig(H);

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% 6) Calculation of the retarded Green's function and the associated
% spectral function
for en = 1:length(Evet);
E = Evet(en);
Gr = 1./(E-E_a+i*eta);
rho(en) = -1/pi*sum(imag(Gr));
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 7) Calculation of the eigeneneregies for the isolated unit cell
E_i = eig(H_0);
rho_a = zeros(1,length(Evet),1);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 8) Calculation of the analytical density of states: sum over N_y chains
rho_a = zeros(1,length(Evet));
for mode = 1:length(E_i);
rho_a = rho_a + 1/pi*real(1./sqrt(4*b_inter^2 - (Evet - E_i(mode)).^2 + eta));
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% 9) Graphic representation of the results
figure(1)
plot(Evet,rho/(N_x+1))
hold on
plot(Evet,rho_a,'r')
if per == 1
title(['Density of states for a tube of N_y = ', num2str(N_y)], 'Fontsize', 15)
else
title(['Density of states for a ribbon of N_y = ', num2str(N_y)], 'Fontsize', 15)
end
xlabel('E[|t|]','Fontsize', 15)
ylabel('DOS[1/|t|]','Fontsize', 15)
legend(['N_x = ',num2str(N_x)],'N_x = \infty')
hold off
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%                                                                                      %
%                                       THE END                                        %
%                                                                                      %
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