

2D square lattice weak periodic potential:

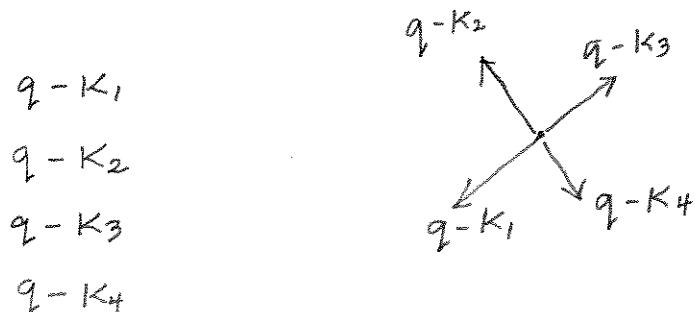
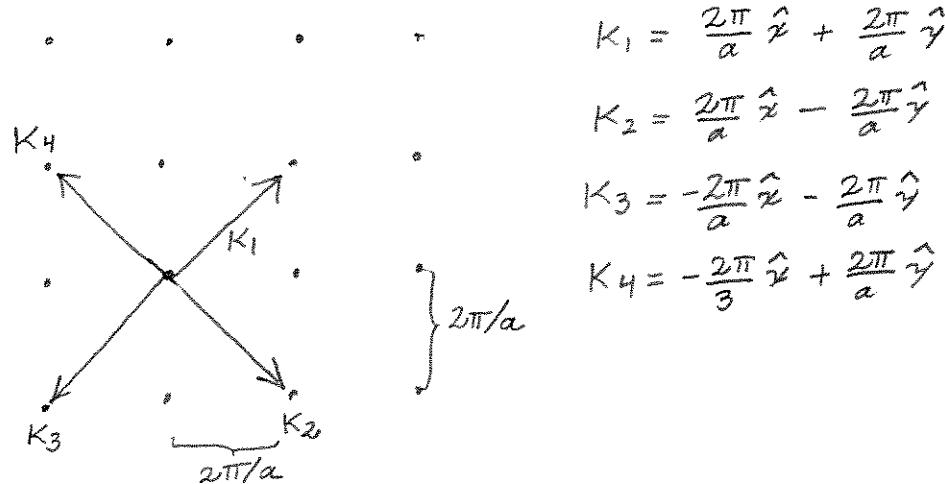
$$\begin{aligned} U(x, y) &= U \cos\left(\frac{2\pi}{a}x\right) \cos\left(\frac{2\pi}{a}y\right) \\ &= \frac{U}{4} (e^{iK_1 \cdot r} + e^{iK_2 \cdot r} + e^{iK_3 \cdot r} + e^{iK_4 \cdot r}) \end{aligned}$$

$$K_1, \dots, K_4 = \pm \frac{2\pi}{a} \hat{x} \pm \frac{2\pi}{a} \hat{y}$$

$$-\frac{\hbar^2 \nabla^2}{2m} \psi + U \psi = E \psi$$

$$\psi = \sum_q c_q e^{iq \cdot r}$$

$$E_q^0 c_q + \frac{U}{4} (c_{q-K_1} + c_{q-K_2} + c_{q-K_3} + c_{q-K_4}) = E c_q$$



2.

$$\begin{pmatrix} \epsilon_q & U/4 & & & \\ U/4 & \epsilon_q^o - K_1 & & & \\ & & U/4 & U/4 & U/4 \\ & & U/4 & \epsilon_q^o - K_2 & \\ & & & & U/4 - K_3 \\ & & & & & U/4 - K_4 \end{pmatrix} \begin{pmatrix} C_0 \\ C_{q-K_1} \\ C_{q-K_2} \\ C_{q-K_3} \\ C_{q-K_4} \end{pmatrix} = E \begin{pmatrix} C_0 \\ C_{q-K_1} \\ C_{q-K_2} \\ C_{q-K_3} \\ C_{q-K_4} \end{pmatrix}$$

In matlab take $a=1$. $\frac{k^2}{2m}=1$. U varies.

first Brillouin zone: reach origin no Bragg plane

2 nd	"	"	:	"	"	"	1	"	"
3 rd	"	"	:	"	"	"	2	"	"
:									
n	"	"	:	"	"	"	n-1	"	"

See mse.ncsu.edu on Google Search for Brillouin zones square lattice.

www.phys.ufl.edu/fermisurface

Structure factor monoatomic lattice w/basis:

$$U(r) = \sum_R \sum_j \phi(r - R - d_j)$$

basis

$$U_K = \frac{1}{V} \int_{\text{cell}} d^3 r e^{-i K \cdot r} \sum_{R,j} \phi(r - R - d_j)$$

$$= \frac{1}{V} \int_{\substack{\text{all} \\ \text{space}}} d^3 r e^{-i K \cdot r} \sum_j \phi(r - d_j)$$

$$= \frac{1}{V} \int_{\substack{\text{all} \\ \text{space}}} d^3 r e^{-i K \cdot (r - d_j)} e^{-i K \cdot d_j} \sum_j \phi(r - d_j)$$

$$= \frac{1}{V} \phi(K) \sum_j e^{-i K \cdot d_j}$$

$$= \frac{1}{V} \phi(K) S_K^*, \text{ where } \phi(K) = \int_{\substack{\text{all} \\ \text{space}}} d^3 r e^{-i K \cdot r} \phi(r)$$

$$S_K = \sum_j e^{i K \cdot d_j}$$

Spin orbit can remove degeneracies, also spin not a good quantum number.

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a = 1;
U = 20.0;

[kx,ky] = meshgrid(pi*(-1:0.05:1)/a);

K1x = 2*pi/a; K1y = 2*pi/a;
K2x = 2*pi/a; K2y = -2*pi/a;
K3x = -2*pi/a; K3y = -2*pi/a;
K4x = -2*pi/a; K4y = 2*pi/a;

Npts = size(kx,1); % Assumes square in k-space
band1 = 0*kx;
band2 = 0*kx;
band3 = 0*kx;
band4 = 0*kx;
band5 = 0*kx;

for mx = 1:Npts,
    for my = 1:Npts,
        qx = kx(mx,my);
        qy = ky(mx,my);
        ep0q = qx^2 + qy^2;
        ep0qK1 = (qx - K1x)^2 + (qy - K1y)^2;
        ep0qK2 = (qx - K2x)^2 + (qy - K2y)^2;
        ep0qK3 = (qx - K3x)^2 + (qy - K3y)^2;
        ep0qK4 = (qx - K4x)^2 + (qy - K4y)^2;
        H = [ ep0q U/4 U/4 U/4 U/4;
              U/4 ep0qK1 0 0 0;
              U/4 0 ep0qK2 0 0;
              U/4 0 0 ep0qK3 0;
              U/4 0 0 0 ep0qK4 ];
        E = sort(eig(H)); % sorting places lowest at 1 position
        band1(mx,my) = E(1);
        band2(mx,my) = E(2);
        band3(mx,my) = E(3);
        band4(mx,my) = E(4);
        band5(mx,my) = E(5);
    end
end

figure(1)
hold off
surf(kx,ky,band1)
hold on
surf(kx,ky,band2)
surf(kx,ky,band3)
hold off

figure(2)
contour(kx,ky,band1)
xlabel('kx')
ylabel('ky')
title('band 1')

figure(3)
contour(kx,ky,band2)
xlabel('kx')
ylabel('ky')
title('band 2')

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