Problem 2

Using the tight-binding (LCAO) approach, compute the energy band formed by atomic s-orbitals in an fcc lattice with a monoatomic basis. Plot the energy vs q along L - Γ - X - U - Γ

```
gamma1 = -1;

Gamma = [0, 0, 0];
X = [2*pi, 0, 0];
L = [pi, pi, pi];
U = [2*pi, pi, 0];
% Since a cancels out when calculating the energy, plus we don't have a
% value to set it to, I'm going to leave it out of this solution.

k_LG = [linspace(L(1), Gamma(1), 100); linspace(L(2), Gamma(2), 100);
linspace(L(3), Gamma(3), 100)];
k_GX = [linspace(G(1), X(1), 100); linspace(Gamma(2), X(2), 100);
linspace(Gamma(3), X(3), 100)];
k_XU = [linspace(X(1), U(1), 100); linspace(X(2), U(2), 100); linspace(X(3), U(3),
100)];
k_UG = [linspace(U(1), Gamma(1), 100); linspace(U(2), Gamma(2), 100);
linspace(U(3), Gamma(3), 100)];

E_LG = 2 * gamma1 * (cos(k_LG(1,:)) + cos(k_LG(2,:)) + cos(k_LG(3,:)));
E_GX = 2 * gamma1 * (cos(k_GX(1,:)) + cos(k_GX(2,:)) + cos(k_GX(3,:)));
E_XU = 2 * gamma1 * (cos(k_XU(1,:)) + cos(k_XU(2,:)) + cos(k_XU(3,:)));
E_UG = 2 * gamma1 * (cos(k_UG(1,:)) + cos(k_UG(2,:)) + cos(k_UG(3,:)));

figure;
hold on;
grid on;
% L -> Gamma
subplot(2, 2, 1);
plot(E_LG, 'b', 'LineWidth', 2);
title('Energy Band vs q: M → Γ');
ylabel('Energy E(q)');

% Gamma -> X
subplot(2, 2, 2);
plot(E_GX, 'g', 'LineWidth', 2);
title('Energy Band vs q: Γ → X');
ylabel('Energy E(q)');

% X -> U
subplot(2, 2, 3);
plot(E_XU, 'r', 'LineWidth', 2);
title('Energy Band vs q: X → M');
xlabel("q (Reciprocal space)");
ylabel('Energy E(q)');
```

```
% U -> Gamma
subplot(2, 2, 4);
plot(E_UG, 'r', 'LineWidth', 2);
title('Energy Band vs q: X → M');
xlabel("q (Reciprocal space)");
ylabel('Energy E(q)');
```