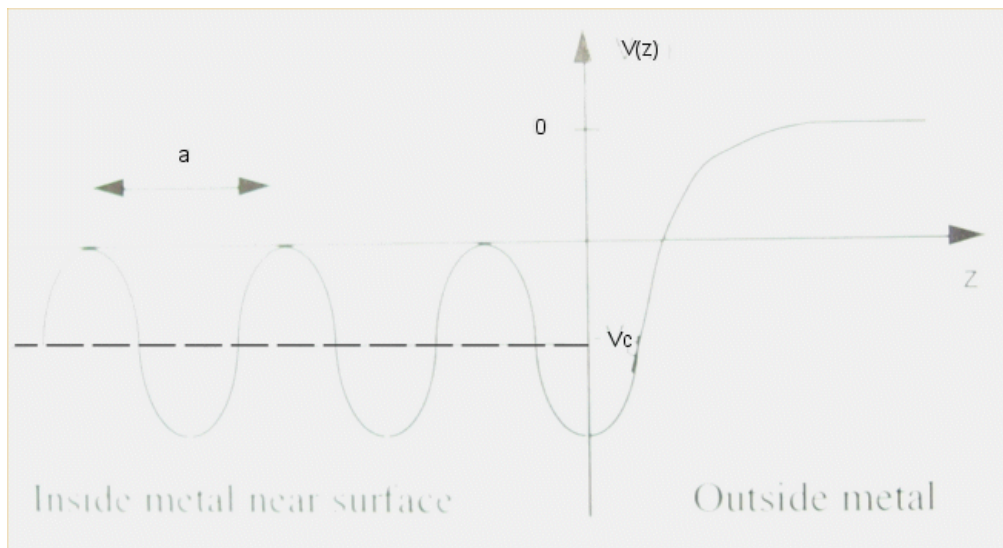


- 1) (Similar to Ashcroft and Mermin problem 18.2) We have seen that the periodicity of a 3D lattice gives rise to energy bands and band gaps. At the surface of a solid, the abrupt end to the periodicity gives rise to surface states, which are real and detectable. In this challenging but technologically important problem, you will examine the quantum mechanical origin of surface states. An approximation of a metal surface including the ionic cores and a surface barrier is given by:



Where  $V(z)$  is a weak periodic potential,

$V(z) = -V_0 + 2V_g \cos gz = -V_0 + V_g [e^{igz} + e^{-igz}]$ , and  $g = \frac{2\pi}{a}$  is the shortest reciprocal lattice vector.

- a) Though in general  $\Psi_k(z)$  and  $V(z)$  can be expressed as the Fourier series of plane waves, assume that two of the plane waves dominate and use this as your trial solution:

$$\Psi_k(z) = \Psi_{10} e^{ikz} + \Psi_{20} e^{i(k-g)z}$$

What is the secular equation, and what are the eigenvalues and eigenfunctions?

Since I may ignore terms outside the Brillouin Zone, I take trial solutions:

$$\Psi_k(z) = \Psi_{10} e^{ikz} + \Psi_{20} e^{i(k-g)z}$$

Ashcroft and Mermin 9,24 gives the secular equation as:

$$\begin{vmatrix} \varepsilon - \varepsilon_k^0 - V_0 & -U_g \\ -U_g^* & \varepsilon - \varepsilon_{k-g}^0 - V_0 \end{vmatrix} = 0$$

Here,  $U_g = V_g$  is the Fourier component of the potential in the given period and

$$\varepsilon_k^0 \equiv \frac{\hbar^2}{2m} k^2 \text{ and } \varepsilon_{k-g}^0 \equiv \frac{\hbar^2}{2m} (k-g)^2.$$

Ashcroft and Mermin 9.26 gives the roots of this equation as:

$$\varepsilon - V_0 = \frac{1}{2} (\varepsilon_k^0 + \varepsilon_{k-g}^0) \pm \sqrt{\left( \frac{\varepsilon_k^0 - \varepsilon_{k-g}^0}{2} \right)^2 + |U_g|^2}$$

In this case, then, I have:

$$\varepsilon - V_0 = \frac{1}{2} \frac{\hbar^2}{2m} (2k^2 - 2gk + g^2) \pm \sqrt{\left( \frac{\hbar^2}{4m} (2k^2 - 2gk + g^2) \right)^2 + V_g^2}$$

This energy appears to be always real inside the bulk solid, assuming that  $k$  is entirely real.

The coefficients of the eigenfunction are rather complex, and will be given by the null space of the matrix above, yielding a ratio between the coefficients in

$$\Psi_k(z) = \Psi_{10} e^{ikz} + \Psi_{20} e^{i(k-g)z}.$$

Using the Eigensystem function in Mathematica to find these coefficients exactly, I see that for the plus combination energy above:

$$E_{k+} : \frac{\Psi_{10}}{\Psi_{20}} = \frac{g\hbar^2(g-2k)m + \sqrt{g^2\hbar^4(g-2k)^2 m^2 + 16m^4 V_g^2}}{4m^2 V_g}$$

For the minus combination,

$$E_{k-} : \frac{\Psi_{10}}{\Psi_{20}} = \frac{g\hbar^2(g-2k)m - \sqrt{g^2\hbar^4(g-2k)^2 m^2 + 16m^4 V_g^2}}{4m^2 V_g}$$

- b) In the interior of the crystal an energy gap arises because of the limitations on the momentum due to the periodicity of the potential. At the surface this restriction is relaxed, leading to the possibility of surface states within the band gap. Under what condition will there be a surface state for this potential?**

A surface state will exist for a particular potential if the matching condition of continuity is obeyed: namely,  $\Psi_{in} = \Psi_{out}$  and also  $\bar{\nabla}\Psi_{in} = \bar{\nabla}\Psi_{out}$ .

I write  $\kappa \equiv k - \frac{g}{2}$ , and then plot energy as a function of this new variable. In this regime, then, I get the symmetric form:

$$\Psi_{\kappa}(z) = \Psi_{10}e^{i\left(\kappa+\frac{g}{2}\right)z} + \Psi_{20}e^{i\left(\kappa-\frac{g}{2}\right)z}$$

Clearly, the wave function outside will obey

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi = E\psi$$

outside, where here  $\psi$  should be exponential in form. However, in order to be decaying in this region under the assumption that the potential outside is  $V(z > 0) = 0$ . Then, it must be the case that  $E(\kappa) < 0$  in order to decay outside. This region is illustrated in the plot below.

Next, it must be the case inside the material that some finite solution exists up to  $z = \frac{a}{2}$  after which point bulk states can be matched. However, imaginary solutions for  $\kappa$  don't satisfy periodic boundary conditions. Then, looking at part (a), I see that with

$$E_{k\pm} : \frac{\Psi_{10}}{\Psi_{20}} = \frac{g\hbar^2(g-2k)m \pm \sqrt{g^2\hbar^4(g-2k)^2m^2 + 16m^4V_g^2}}{4m^2V_g}$$

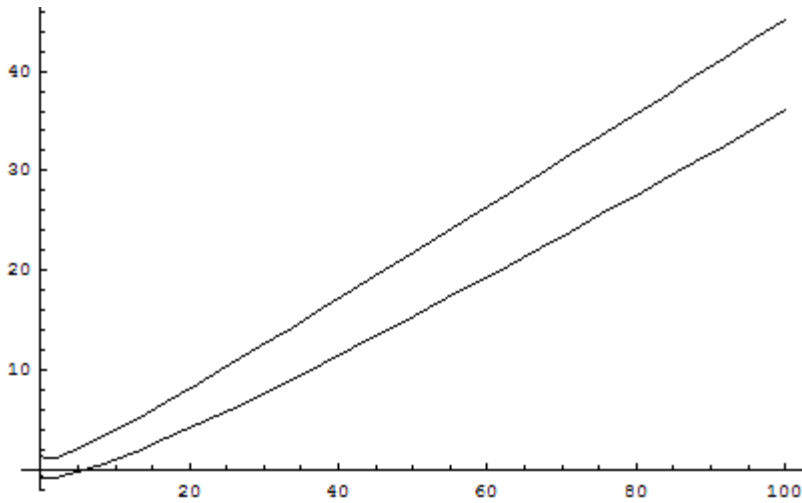
$$4g^2\hbar^4\kappa^2m^2 + 16m^4V_g^2 > 0$$

$$g^2\frac{\hbar^4}{4m^2}\kappa^2 < V_g^2$$

$$0 < \left| g^2\frac{\hbar^4}{4m^2}\kappa^2 \right| < V_g$$

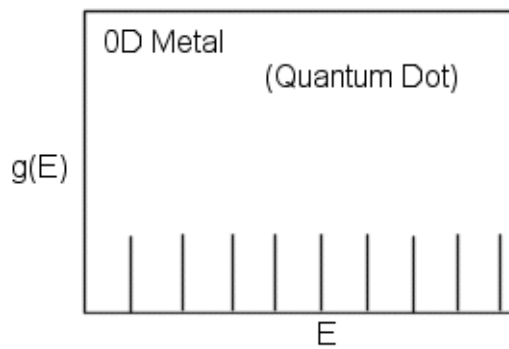
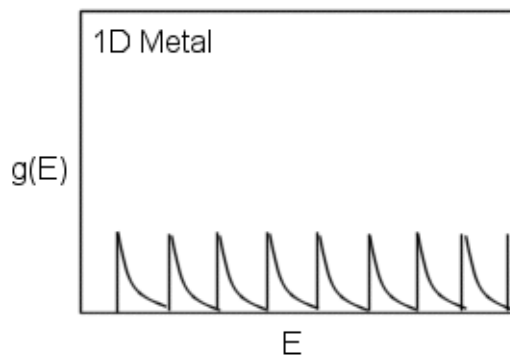
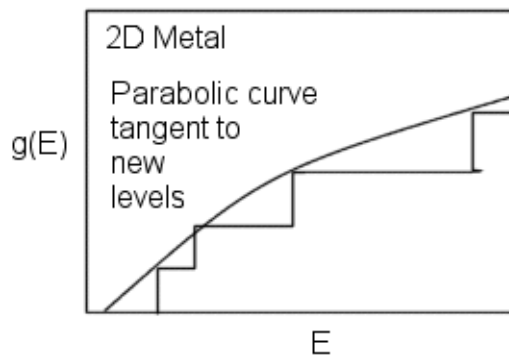
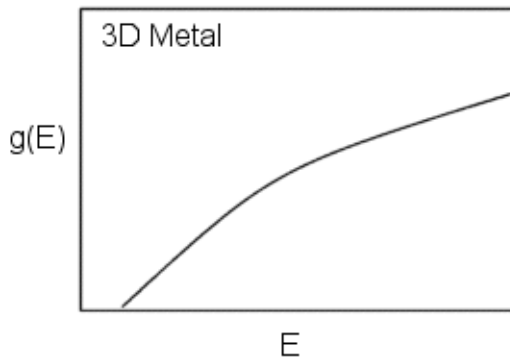
as my other condition.

Plotting  $E - V_0$  vs  $\kappa^2$  with sample values, I obtain from this expression:



2)

- a) Make qualitative sketches of the density of states function  $g(E)$  versus the energy  $E$  for the free electron model of a three-dimensional (3D), 2D, 1D and 0D metal.
- b) For the 2D metal, label the graph of  $g(E)$  qualitatively.



In the 2D metal graph, each step must have height  $\frac{m}{\pi\hbar^2}$  and the spacings are at

$$\varepsilon_1, \varepsilon_2 = 4\varepsilon_1, \varepsilon_3 = 9\varepsilon_1, \dots$$

- c) **Many applications of quantum transport involve a two-dimensional electron gas (2DEG) that is placed in a perpendicular magnetic field. With an external magnetic field, the Hamiltonian contains an extra term with the vector potential  $\mathbf{A}$ :**

$$\hat{H} = \frac{1}{2m} (\vec{p} - e\vec{A})^2$$

**If the electrons move in the xy-plane, we can use the Landau gauge with**

**$\hat{A} = (-By, 0, 0)$  so that the field  $B$  is in the z direction.**

$$\hat{H}\Psi = \frac{\hbar^2}{2m} \left[ \left( \frac{1}{i} \frac{\partial}{\partial x} + \frac{eB}{\hbar} y \right)^2 - \frac{\partial^2}{\partial y^2} \right] \Psi = E\Psi$$

**with momentum conserved in the x-direction, use a trial solution  $\Psi \propto e^{ikx}\Phi(y)$ , and solve for  $\Phi(y)$  and the allowed energies  $E_n$ .**

First I take the trial solution and obtain

$$\frac{\hbar^2}{2m} \left[ \left( k + \frac{eB}{\hbar} y \right)^2 - \frac{\partial^2}{\partial y^2} \right] \Psi = E\Psi$$

Define:  $l \equiv \sqrt{\frac{\hbar}{eB}}$

$$\frac{\hbar^2}{2m} \left[ \left( k + \frac{y}{l^2} \right)^2 - \frac{\partial^2}{\partial y^2} \right] \Psi = E\Psi$$

$$\left[ \left( lk + \frac{y}{l} \right)^2 - l^2 \frac{\partial^2}{\partial y^2} \right] \Psi = l^2 \frac{2mE}{\hbar^2} \Psi$$

Define:

$$Y \equiv \left( lk + \frac{y}{l} \right)$$

$$K \equiv \frac{2mEl^2}{\hbar^2}$$

$$\frac{\partial}{\partial Y} = \frac{\partial y}{\partial Y} \frac{\partial}{\partial y} = l \frac{\partial}{\partial y}$$

$$\left[ Y^2 - \frac{\partial^2}{\partial Y^2} \right] \Psi = K \Psi$$

Now I consider series solutions with:  $\Phi(Y) = e^{-\frac{Y^2}{2}} \left[ \sum_{n=0}^{\infty} a_n Y^n \right]$ . Then:

$$\frac{d^2 \Phi}{dY^2} = e^{-\frac{Y^2}{2}} \left( \frac{d^2}{dY^2} - 2Y \frac{d}{dY} + (Y^2 - 1) \right) \left[ \sum_{n=0}^{\infty} a_n Y^n \right]$$

Now I have:

$$\left[ Y^2 - \frac{\partial^2}{\partial Y^2} - K \right] \left[ \sum_{n=0}^{\infty} a_n Y^n \right] = 0$$

$$\left[ Y^2 - \left( \frac{d^2}{dY^2} - 2Y \frac{d}{dY} + (Y^2 - 1) \right) - K \right] \left[ \sum_{n=0}^{\infty} a_n Y^n \right] = 0$$

$$\left[ \frac{d^2}{dY^2} - 2Y \frac{d}{dY} + (K - 1) \right] \left[ \sum_{n=0}^{\infty} a_n Y^n \right] = 0$$

and each term of this must vanish separately. Thus, I have:

$$n = 0: (K - 1)a_0 + 2a_2 = 0$$

$$n > 0: (K - 1)a_n + (n + 1)(n + 2)a_{n+2} - 2na_n = 0$$

Now on inspection I see that the even and odd portions of this function don't mix, so that I may write:

$$\Phi_{\text{even}}(y) = \sum_{n=0}^{\infty} a_{2n} y^{2n}$$

$$\Phi_{\text{odd}}(y) = \sum_{n=0}^{\infty} a_{2n+1} y^{2n+1}$$

Now I see that for these series to converge, they must eventually terminate. Let  $N$  represent the highest-order nonzero coefficient. Considering even solutions first:

$$N = 0: \frac{a_2}{a_0} = 0 = \frac{K - 1}{2} \rightarrow K_0 = 1 \rightarrow E_0 = \frac{\hbar^2}{2ml^2}$$

$$N > 0: (K - 1 - 2N)a_N + (N + 1)(N + 2)a_{N+2} = 0 \rightarrow \frac{a_{N+2}}{a_N} = \frac{(2N + 1 - K_N)}{(N + 1)(N + 2)}$$

$$\therefore 2N + 1 - K_N = 0 \rightarrow K_N = 2N + 1 \rightarrow E_N = \frac{(2N + 1)\hbar^2}{2ml^2}$$

Summary:

So I see then that the solutions contain Hermite polynomials:

$$\Phi(Y) = e^{-\frac{Y^2}{2}} \left[ \sum_{n=0}^{\infty} a_n Y^n \right]$$

$$\text{with } Y \equiv \left( lk + \frac{y}{l} \right) \quad l \equiv \sqrt{\frac{\hbar}{eB}}$$

exist such that  $E_N = \frac{(2N+1)\hbar^2}{2ml^2}$  with coefficients  $a_n$  given for excited state  $N$  by :

$$n = 0: (N-1)a_0 + 2a_2 = 0$$

$$n > 0: (N-1)a_n + (n+1)(n+2)a_{n+2} - 2na_n = 0$$

Here, I have defined  $K_N \equiv \frac{2mE_N l^2}{\hbar^2} = 2N + 1$ .

**d) Consider the implications for the density of states. What is the constraint on  $k_x^2$  and  $k_y^2$  based on the energy found in part c?**

By  $k_x^2$  and  $k_y^2$ , we mean the components of the wave-vector for the linear combinations of solutions indexed in this direction.

Recall that  $E = \frac{\hbar^2 k^2}{2m}$ , for a free propagating particle, and so for such a particle in a free electron gas not in a field I get

$$g \left( E = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m} \right) = \sum_n \theta \left( E_n - \frac{\hbar^2 (k_x^2 + k_y^2)}{2m} \right).$$

This gives rise to the behavior shown in part (a), as the number circumference of available states increases in terms of wave vector. However, here we speak of a free electron gas in a strong magnetic field. Thus, in part (c) the states appear to have collapsed to

$$E_N = \frac{(2N+1)\hbar^2}{2ml^2}.$$

Comparing this to the totally free electron, I expect something akin to

$$k_1^2 + k_2^2 = \frac{(2N+1)}{l^2}$$

for energy states  $N$ .

- e) For a given quantum number  $n$ , if the 2DEG has dimension  $L_x$  in the x-direction, what is the geometrical constraint on  $k$ ? If the 2DEG has dimension  $L_y$  in the y-direction, what is the maximum value for  $k$ ?

If the 2D electron gas has dimension  $L_x$  in the x-direction, then it must be the case that  $e^{ikx}$  has  $L_x = \frac{2\pi n}{k}$  so that the wave function might vanish at the border of the gas.

Next I consider the dimension  $L_y$ . Since the ground state solution of  $\Phi(Y)$  is a Gaussian, it vanishes only in the infinite limit. Then I see that this function must be at least in its second excited state for finite dimensions  $L_y$  so that it may vanish at two borders.

Now I see that I can obtain a minimum on  $k$  based on this boundary condition:

$$\frac{\hbar^2(k_x^2 + k_y^2)}{2m} \rightarrow |k| > \sqrt{\frac{(2N+1)}{l^2}}$$

In terms of a maximum, I can examine the Gaussian from part c:

$$\Phi(Y) = e^{-\frac{Y^2}{2}} \left[ \sum_{n=0}^{\infty} a_n Y^n \right], \quad Y \equiv \left( lk + \frac{y}{l} \right) \quad l \equiv \sqrt{\frac{\hbar}{eB}}$$

I see that the center of my Gaussian is shifted by  $lk$ , and so in order for the peak corresponding to the particle's average position to remain within the boundary, I must have (assuming that the length of the box is centered at the origin):

$$lk < \frac{L_y}{2l} \rightarrow 2l^2 k < L_y$$

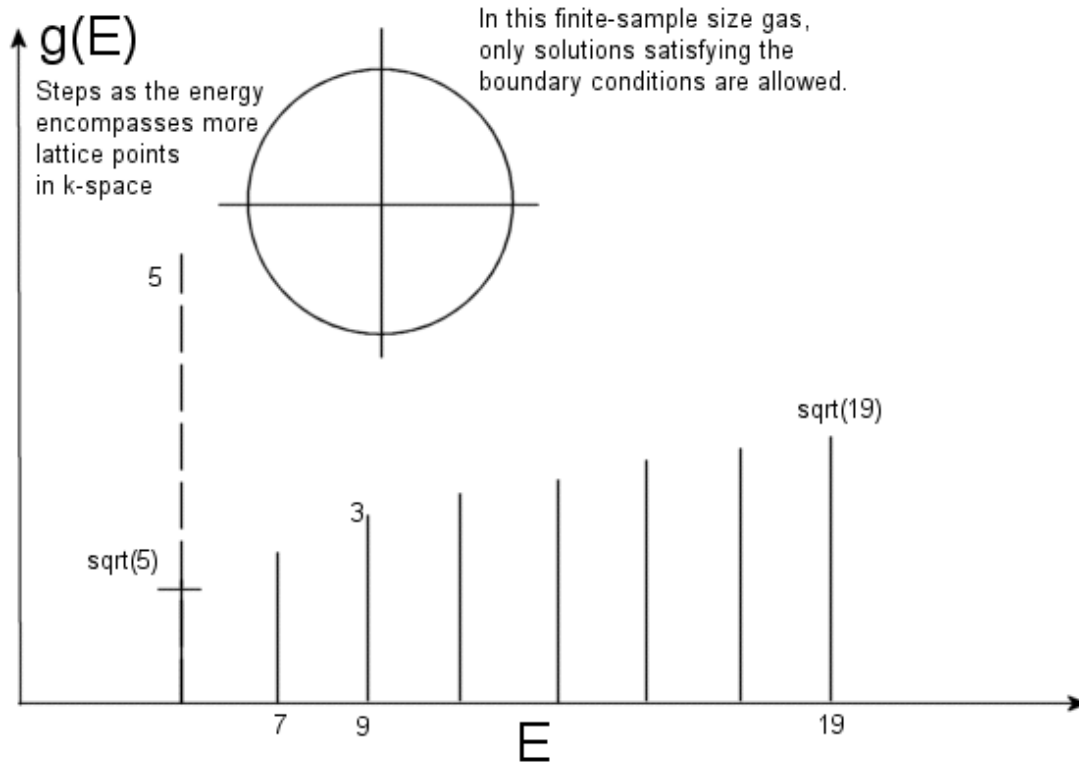
Here I have assumed that the box's length is centered at the origin.

- f) Combine the two expressions from part (d) to determine the maximum number of states within this energy level. For a 2D system, the number density  $N$  will be given by the number of states divided by  $L_x L_y$ . Make a quantitative, labeled plot of the 2D density of states for a free electron metal in a perpendicular magnetic field.

The constraint from (d) that

$$g\left(E = \frac{\hbar^2(k_x^2 + k_y^2)}{2m}\right) = \sum_n \delta\left(E_n - \frac{\hbar^2(k_x^2 + k_y^2)}{2m}\right)$$

Including spin degeneracy, there are two of each such states; however, in a strong perpendicular magnetic field it is likely that the splitting is substantial (so that one is possibly ignored).



Above,  $E$  has units of  $\frac{\hbar^2}{2ml^2}$  and  $g(E)$  is roughly in units of  $2\pi$  (corresponding to the circumference of a circle traced by  $k$ ). The allowed energies correspond to a value  $k_x^2 + k_y^2$  of this circumference, and I have assumed proportionality here. Thus, I see that what is a staircase-like function in the free case is collapsed to these levels in a strong magnetic field.

3)

- a) **Eli Yablonovich described how the concepts of electronic band structure could be applied to design a material with a photonic band gap. Suppose you wanted a “phononic band gap” material. What interesting properties might it have? How would you design its structure and how might you determine if it has a phononic band gap?**

First, it is important to note why the photonic band gap exists: by introducing small spheres of a material with a sufficiently differing index of refraction. Glossing over the details, Yablonovich and his group were able to cause microwaves whose wave vectors coincided nearly with the reciprocal lattice vector and nearly as a multiple of the magnitude of the material’s lattice vector to experience a resonance and be dispersed unlike other microwaves.

This is a bit different from how phonons work: whereas a photon is a separate particle, the acoustic phonons arise from the motion of the atoms corresponding to the lattice sites within the material. As long as the material has translational invariance, the phonons will propagate themselves. However, an extremely disordered material might disperse the phonons much more effectively than a very well-ordered one.

Certainly, a phononic band gap material would be useful for such needs as selective sound-dampening, for example producing ear-protection equipment that would allow one to nonetheless hear what co-workers are saying.

It is important to note that a linear chain of atoms does exhibit a band gap between “acoustic phonons” and “optical phonons”, where acoustic phonons arise from translational invariance and optical phonons are due to adjacent particles oscillating out of phase. This can be easily shown by assuming a linear “ring” of sites. However, this band gap is not consistent across all directions in a 3D lattice. Thus, one might be able to produce a phononic band gap metamaterial by stretching extraordinarily fine wires—an atom thick if possible--of some material in a vacuum between two opposing surfaces (for absorption and transmission).

Another approach is to produce a metamaterial with periodic densities (since sound is affected by density rather than by index of refraction), and then apply the same techniques as with a microwave band gap metamaterial, producing a lattice of spheres of a greater density.

**b) In Evgeny Tsymbal’s paper on spin polarization effects at the Co-oxide surface, the authors noted that only  $k_{\parallel}$  was conserved. Explain why this is true.**

Inspection of the surface would show that there is most definitely not translational invariance perpendicular to the surface into a separate material, but it is clear that there is translational invariance in terms of moving parallel to the surface. Thus, this was a logical parameter to use for calculations.