

I give numbers to the constants. In the units given (hbar/2m - where I take hbar in ev*s, because that is what's on the graph)

$$Ael := - \frac{4.29 \cdot h^2}{2 \cdot 9.109 \cdot 10^{-31}} \quad -1.020206584 \quad (1)$$

$$h := 6.582119514 \cdot 10^{-16} \quad 6.582119514 \cdot 10^{-16} \quad (2)$$

$$Ag := - \frac{13.38 \cdot h^2}{2 \cdot 9.109 \cdot 10^{-31}} \quad -3.181903051 \quad (3)$$

$$Bel := \frac{0.68 \cdot h^2}{2 \cdot 9.109 \cdot 10^{-31}} \quad 0.1617110669$$

$$Bg := \frac{8.48 \cdot h^2}{2 \cdot 9.109 \cdot 10^{-31}} \quad 2.016632128$$

$$Cel := \frac{4.87 \cdot h^2}{2 \cdot 9.109 \cdot 10^{-31}} \quad 1.158136611 \quad (6)$$

$$Cg := \frac{13.15 \cdot h^2}{2 \cdot 9.109 \cdot 10^{-31}} \quad 3.127206661 \quad (7)$$

$$ds := 0.044 \quad 0.044 \quad (8)$$

$$dg := 0.29 \quad 0.29 \quad (9)$$

$$a := 1 \quad 1 \quad (10)$$

Put the numbers in formula (kx=k, ky and kz =0)

$$es(K) := -ds + Ael \cdot K^2 \quad K \rightarrow -ds + Ael K^2 \quad (11)$$

$$eg(K) := -dg + Ag^2 \cdot K^2 \quad K \rightarrow -dg + Ag^2 K^2 \quad (12)$$

$$e(K) := Ael \cdot K^2 + (Bel^2 \cdot K^4)^{\frac{1}{2}} \quad K \rightarrow Ael K^2 + \sqrt{Bel^2 K^4} \quad (13)$$

$$egl(K) := Ag \cdot K^2 + (Bg^2 K^4)^{\frac{1}{2}}$$

$$e2(K) := AeI \cdot K^2 - (BeI^2 \cdot K^4)^{\frac{1}{2}} \quad K \rightarrow Ag K^2 + \sqrt{Bg^2 K^4} \quad (14)$$

$$K \rightarrow AeI K^2 - \sqrt{BeI^2 K^4} \quad (15)$$

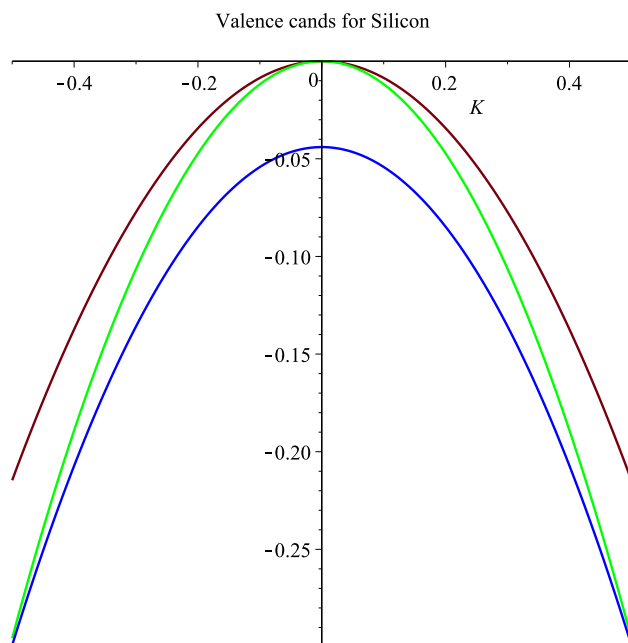
$$eg2(K) := Ag^2 \cdot K^2 - (Bg^2 \cdot K^4)^{\frac{1}{2}} \quad K \rightarrow Ag^2 K^2 - \sqrt{Bg^2 K^4} \quad (16)$$

$$A := plot(e(K), K=-0.5..0.5) \quad PLOT(...) \quad (17)$$

$$B := plot(e2(K), K=-0.5..0.5, color=green) \quad PLOT(...) \quad (18)$$

$$C := plot(es(K), K=-0.5..0.5, color=blue) \quad PLOT(...) \quad (19)$$

$$display(A, B, C)$$



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Ag := plot(eg(K), K=-0.3..0.3, color=blue)
                                PLOT(...)
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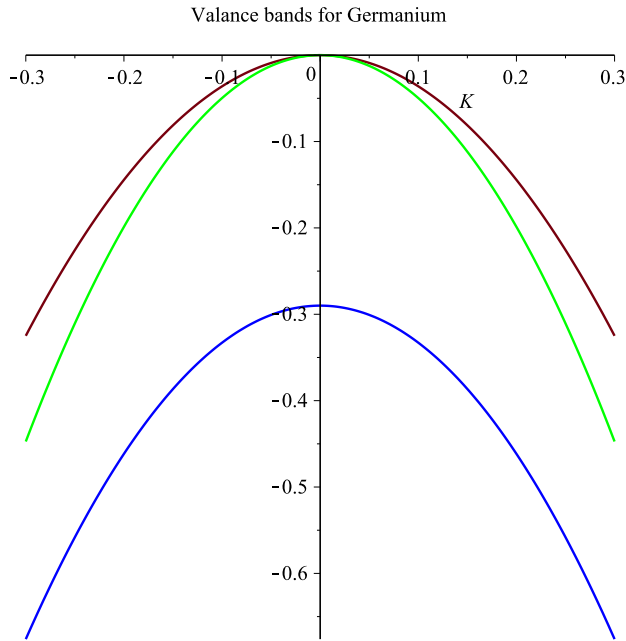
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Bg := plot(eg1(K), K=-0.3..0.3)
                                PLOT(...)
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Cg := plot(eg2(K), K=-0.3..0.3, color=green)
                                PLOT(...)
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display(Ag, Bg, Cg)
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(21)

(22)



b)for that part I need K in tems of kx and ky.

$$Kt := \sqrt{kx^2 + ky^2 + kz^2}$$

$$\sqrt{kx^2 + ky^2} \quad (23)$$

$$kz := 0$$

$$0 \quad (24)$$

$$es(kx, ky) := Ae1 \cdot Kt^2 + (Be1^2 \cdot Kt^4 + Ce1^2 \cdot kx^2 \cdot ky^2)^{\frac{1}{2}}$$

$$(kx, ky) \rightarrow Ae1 Kt^2 + \sqrt{Be1^2 Kt^4 + Ce1^2 kx^2 ky^2} \quad (25)$$

$$es2(kx, ky) := Ae1 \cdot Kt^2 - (Be1^2 \cdot Kt^4 + Ce1^2 \cdot kx^2 \cdot ky^2)^{\frac{1}{2}}$$

$$(kx, ky) \rightarrow Ae1 Kt^2 - \sqrt{Be1^2 Kt^4 + Ce1^2 kx^2 ky^2} \quad (26)$$

$$es3(kx, ky) := -ds + Ae1 \cdot Kt^2$$

$$(kx, ky) \rightarrow Ae1 Kt^2 - ds \quad (27)$$

$$A2 := plot3d(es(kx, ky), kx=-0.3..0.3, ky=-0.3..0.3, color=blue)$$

$$PLOT3D(...) \quad (28)$$

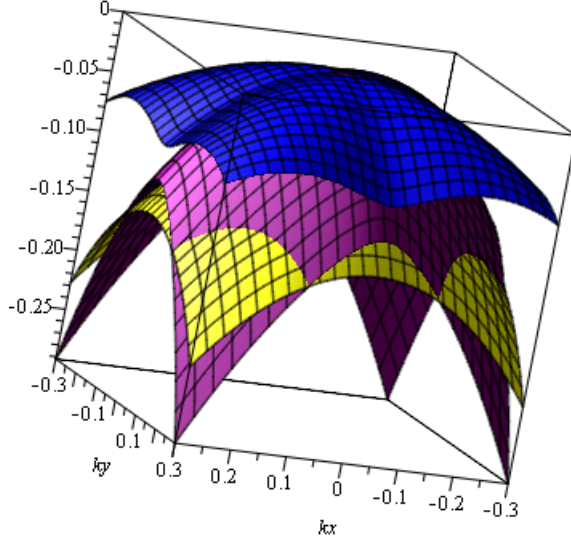
$$B2 := plot3d(es2(kx, ky), kx=-0.3..0.3, ky=-0.3..0.3, color=purple)$$

PLOT3D(...) (29)

$C2 := \text{plot3d}(\text{es3}(kx, ky), kx=-0.3..0.3, ky=-0.3..0.3, \text{color}=\text{yellow})$

PLOT3D(...) (30)

$\text{display}(A2, B2, C2)$



$$\begin{aligned} \text{eg}(kx, ky) &:= Ag \cdot Kt^2 + (Bg^2 \cdot Kt^4 + Cg^2 \cdot kx^2 \cdot ky^2)^{\frac{1}{2}} \\ &\quad (kx, ky) \rightarrow Ag Kt^2 + \sqrt{Bg^2 Kt^4 + Cg^2 kx^2 ky^2} \end{aligned} \quad (31)$$

$$\begin{aligned} \text{eg2}(kx, ky) &:= Ag \cdot Kt^2 + (Bg^2 \cdot Kt^4 + Cg^2 \cdot kx^2 \cdot ky^2)^{\frac{1}{2}} \\ &\quad (kx, ky) \rightarrow Ag Kt^2 + \sqrt{Bg^2 Kt^4 + Cg^2 kx^2 ky^2} \end{aligned} \quad (32)$$

$$\begin{aligned} \text{eg3}(kx, ky) &:= -dg + Ag \cdot Kt^2 \\ &\quad (kx, ky) \rightarrow Ag Kt^2 - dg \end{aligned} \quad (33)$$

$$\begin{aligned} A3 &:= \text{plot3d}(\text{eg}(kx, ky), kx=-0.5..0.5, ky=-0.5..0.5, \text{color}=\text{blue}) \\ &\quad \text{PLOT3D(...)} \end{aligned} \quad (34)$$

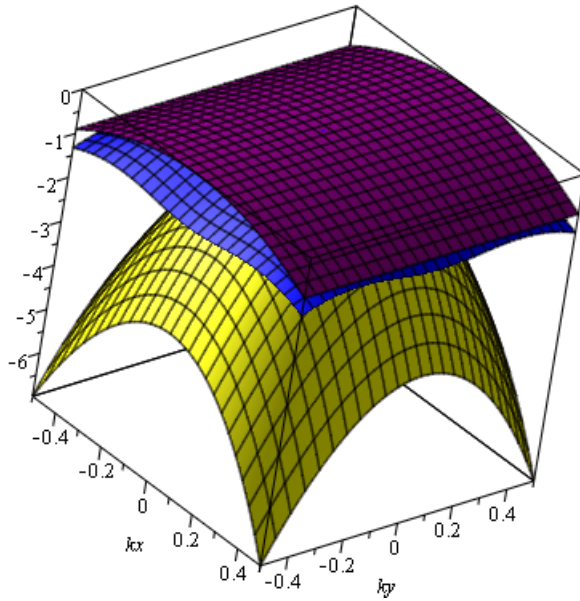
$$\begin{aligned} B3 &:= \text{plot3d}(\text{eg1}(kx, ky), kx=-0.5..0.5, ky=-0.5..0.5, \text{color}=\text{purple}) \\ &\quad \text{PLOT3D(...)} \end{aligned} \quad (35)$$

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C3 := plot3d(eg3(kx, ky), kx=-0.5..0.5, ky=-0.5..0.5, color=yellow)
      PLOT3D(...)
display(A3, B3, C3)

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(36)



c) To calculate effective mass we use equation (29) But plug in constants without putting the m value in it, so our answer is in terms of m .

$$A_h := - \frac{4.29 \cdot h^2}{2 \cdot m} \quad - \frac{9.293061771 \cdot 10^{-31}}{m} \quad (37)$$

$$B_h := \frac{0.68 \cdot h^2}{2 \cdot m} \quad \frac{1.473026108 \cdot 10^{-31}}{m} \quad (38)$$

$$C_h := \frac{4.87 \cdot h^2}{2 \cdot m}$$

$$\frac{1.054946639 \cdot 10^{-30}}{m} \quad (39)$$

$$A_{hg} := -\frac{13.38 \cdot h^2}{2 \cdot m} - \frac{2.898395489 \cdot 10^{-30}}{m} \quad (40)$$

$$B_{hg} := \frac{8.48 \cdot h^2}{2 \cdot m} \frac{1.836950206 \cdot 10^{-30}}{m} \quad (41)$$

$$C_{hg} := \frac{13.15 \cdot h^2}{2 \cdot m} \frac{2.848572547 \cdot 10^{-30}}{m} \quad (42)$$

$$mh := \left(\frac{\frac{d}{dK} \left(\frac{d}{dK} (Ah \cdot K^2 + Bh \cdot K^2) \right)}{h^2} \right)^{-1} -0.2770083102 \, m \quad (43)$$

$$mh2 := \left(\frac{\frac{d}{dK} \left(\frac{d}{dK} (Ah \cdot K^2 - Bh \cdot K^2) \right)}{h^2} \right)^{-1} -0.2012072434 \, m \quad (44)$$

$$mhg := \left(\frac{\frac{d}{dK} \left(\frac{d}{dK} (A_{hg} \cdot K^2 + B_{hg} \cdot K^2) \right)}{h^2} \right)^{-1} -0.2040816328 \, m \quad (45)$$

$$mhg2 := \left(\frac{\frac{d}{dK} \left(\frac{d}{dK} (A_{hg} \cdot K^2 - B_{hg} \cdot K^2) \right)}{h^2} \right)^{-1} -0.04574565415 \, m \quad (46)$$

d) $k_x=k_y=k_z$, so $K=\sqrt{3} \cdot k_x$; also if I put A_h and etc with m variable in it - maple gives me pretty messy answer so the answers for these are the number $\cdot m$.

$$mh3 := evalf \left(\left(\frac{\frac{d}{dK} \left(\frac{d}{dK} \left(Ah \cdot \sqrt{3} \cdot K^2 + \sqrt{3} \cdot K^2 \cdot (Bh^2 + Ch^2)^{\frac{1}{2}} \right) \right)}{h^2} \right) \right)^{-1} \right) 0.9204539253 \quad (47)$$

$$mh4 := evalf \left(\left(\frac{\frac{d}{d K} \left(\frac{d}{d K} \left(Ah \cdot \sqrt{3} \cdot K^2 - \sqrt{3} \cdot K^2 \cdot (Bh^2 + Ch^2)^{\frac{1}{2}} \right) \right)}{h^2} \right)^{-1} \right) \right)$$

-0.06270608192

(48)

$$mhg3 := evalf \left(\left(\frac{\frac{d}{d K} \left(\frac{d}{d K} \left(Ahg \cdot \sqrt{3} \cdot K^2 + \sqrt{3} \cdot K^2 \cdot (Bh^2 + Ch^2)^{\frac{1}{2}} \right) \right)}{h^2} \right)^{-1} \right) \right)$$

-0.06822249732

(49)

$$mhg4 := evalf \left(\left(\frac{\frac{d}{d K} \left(\frac{d}{d K} \left(Ahg \cdot \sqrt{3} \cdot K^2 - \sqrt{3} \cdot K^2 \cdot (Bh^2 + Ch^2)^{\frac{1}{2}} \right) \right)}{h^2} \right)^{-1} \right) \right)$$

-0.03155394511

(50)