Berry Curvature for Graphene

In[25]:=
```
<< MaTeX` (*Loading a MaTex package for LaTex formating*)
```

Graphene Hamiltonian

In[41]:=
```
MaTeX["\\begin{pmatrix}
     \\frac{\\Delta}{2} & q_x \\tau_z -i q_y \\\\
     q_x \\tau_z +i q_y & -\\frac{\\Delta}{2}
\\end{pmatrix}", Magnification → 2]
```

Out[41]=
$$\begin{pmatrix} \frac{\Delta}{2} & q_x \tau_z - i q_y \\ q_x \tau_z + i q_y & -\frac{\Delta}{2} \end{pmatrix}$$

In[44]:= H = {{0, τ_z * q_x - i * q_y}, {τ_z * q_x + i * q_y, 0}} + $\frac{\Delta}{2}$ * {{1, 0}, {0, -1}} (*Hamiltonian*)

Out[44]= $\left\{\left\{\frac{\Delta}{2}, -i\, q_y + q_x\, \tau_z\right\}, \left\{i\, q_y + q_x\, \tau_z, -\frac{\Delta}{2}\right\}\right\}$

In[45]:=
```
H // MatrixForm
```

Out[45]//MatrixForm=
$$\begin{pmatrix} \frac{\Delta}{2} & -i\, q_y + q_x\, \tau_z \\ i\, q_y + q_x\, \tau_z & -\frac{\Delta}{2} \end{pmatrix}$$

Eigenvalues and Eigenvectors

Eigenvalues

```
eig = Eigenvalues[H] (*Complete eigenvalues*)
```

Out[46]= $\left\{-\frac{1}{2}\sqrt{\Delta^2 + 4\, q_y^2 + 4\, q_x^2\, \tau_z^2}, \frac{1}{2}\sqrt{\Delta^2 + 4\, q_y^2 + 4\, q_x^2\, \tau_z^2}\right\}$

E_- = eig[[1]] (*Lower energy *)

Out[49]= $-\frac{1}{2}\sqrt{\Delta^2 + 4\, q_y^2 + 4\, q_x^2\, \tau_z^2}$

In[51]:= E_+ = eig[[2]] (*Upper energy *)

Out[51]= $\frac{1}{2}\sqrt{\Delta^2 + 4\, q_y^2 + 4\, q_x^2\, \tau_z^2}$

In[56]:= δE = E_+ - E_- (*Difference in energy*)

Out[56]= $\sqrt{\Delta^2 + 4\, q_y^2 + 4\, q_x^2\, \tau_z^2}$

Eigenvectors

In[59]:=
```
ev = Eigenvectors[H]
```

Out[59]= $\left\{\left\{\frac{i\left(-\Delta+\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)}{2\left(q_y-i q_x \tau_z\right)}, 1\right\}, \left\{-\frac{i\left(\Delta+\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)}{2\left(q_y-i q_x \tau_z\right)}, 1\right\}\right\}$

```
(*Inorder simplify the above expression we make a few substitutions here *)
```

In[60]:=
$\gamma = \sqrt{\Delta^2 + 4 q_y^2 + 4 q_x^2 \tau_z^2}$

$\eta = 2\left(q_y - i q_x \tau_z\right)$

$\eta_c = 2\left(q_y + i q_x \tau_z\right)$

norm = FullSimplify[$\eta * \eta_c$]

Out[60]= $\sqrt{\Delta^2 + 4 q_y^2 + 4 q_x^2 \tau_z^2}$

Out[61]= $2\left(q_y - i q_x \tau_z\right)$

Out[62]= $2\left(q_y + i q_x \tau_z\right)$

Out[63]= $4\left(q_y^2 + q_x^2 \tau_z^2\right)$

Eigenvectors to be used to find Berry Curvature

In[194]:=
```
MaTeX["|n\\rangle=\\begin{pmatrix}
     \\frac{-i(\\Delta + \\gamma)}{\\eta}  \\\\
     1
\\end{pmatrix}", Magnification → 2]
MaTeX["\\langle n|=\\begin{pmatrix}
     \\frac{i(\\Delta + \\gamma)}{\\eta^*} & 1
\\end{pmatrix}", Magnification → 2]
MaTeX["|n^\\prime\\rangle=\\begin{pmatrix}
     \\frac{i(-\\Delta + \\gamma)}{\\eta}  \\\\
     1
\\end{pmatrix}", Magnification → 2]
MaTeX["\\langle n^\\prime|=\\begin{pmatrix}
     \\frac{-i(-\\Delta + \\gamma)}{\\eta^*} & 1
\\end{pmatrix}", Magnification → 2]
```

Out[194]= $$|n\rangle=\begin{pmatrix} \frac{-i(\Delta+\gamma)}{\eta} \\ 1 \end{pmatrix}$$

Out[195]= $$\langle n|=\begin{pmatrix} \frac{i(\Delta+\gamma)}{\eta^*} & 1 \end{pmatrix}$$

Out[196]= $$|n^\prime\rangle=\begin{pmatrix} \frac{i(-\Delta+\gamma)}{\eta} \\ 1 \end{pmatrix}$$

Out[197]= $$\langle n^\prime|=\begin{pmatrix} \frac{-i(-\Delta+\gamma)}{\eta^*} & 1 \end{pmatrix}$$

In[205]:=
```
nKet = Transpose[{{-(i (Δ + γ))/η, 1}}]
nBra = {{(i (Δ + γ))/η_c, 1}}
npKet = Transpose[{{(i (-Δ + γ))/η, 1}}]
npBra = {{(-i (-Δ + γ))/η_c, 1}}
```

Out[205]= $\left\{\left\{-\frac{i\left(\Delta+\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)}{2\left(q_y-i q_x \tau_z\right)}\right\},\{1\}\right\}$

Out[206]= $\left\{\left\{\frac{i\left(\Delta+\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)}{2\left(q_y+i q_x \tau_z\right)}, 1\right\}\right\}$

Out[207]= $\left\{\left\{\frac{i\left(-\Delta+\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)}{2\left(q_y-i q_x \tau_z\right)}\right\},\{1\}\right\}$

Out[208]= $\left\{\left\{-\frac{i\left(-\Delta+\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)}{2\left(q_y+i q_x \tau_z\right)}, 1\right\}\right\}$

```
prodn = FullSimplify[nBra.nKet] (*inner product of n. <n|n>*)
prodnp = FullSimplify[npBra.npKet](*inner product of np. <np|np>*)
```

Out[211]= $\left\{\left\{1+\frac{\left(\Delta+\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)^2}{4\left(q_y^2+q_x^2 \tau_z^2\right)}\right\}\right\}$

Out[212]= $\left\{\left\{1+\frac{\left(\Delta-\sqrt{\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2}\right)^2}{4\left(q_y^2+q_x^2 \tau_z^2\right)}\right\}\right\}$

In[214]:=
```
norm = FullSimplify[(Sqrt[1/(prodnp)] * Sqrt[1/(prodn)])^2] (*Normalisation
  for both the eigenvectors. It can be broken into two parts A and B *)
```

Out[214]= $\left\{\left\{\frac{1}{4}-\frac{\Delta^2}{4\left(\Delta^2+4 q_y^2+4 q_x^2 \tau_z^2\right)}\right\}\right\}$

In[240]:=
```
MaTeX["\\Omega = i\\frac{\\left\\langle
n\\middle|\\frac{{\\partial}H}{{\\partial}R^{\\mu}}\\middle|n'\\right\\rangle\\
   left\\langle
n'\\middle|\\frac{{\\partial}H}{{\\partial}R^{\\nu}}\\middle|n\\right\\rangle-
   \\left\\langle
n\\middle|\\frac{{\\partial}H}{{\\partial}R^{\\nu}}\\middle|n'\\right\\rangle
   \\left\\langle
n'\\middle|\\frac{{\\partial}H}{{\\partial}R^{\\mu}}\\middle|n\\right\\rangle}
   {(\\epsilon_n - \\epsilon_n')^2}", Magnification → 1.5]
```

Out[240]=
$$\Omega = i\frac{\left\langle n\middle|\frac{\partial H}{\partial R^{\mu}}\middle|n'\right\rangle\left\langle n'\middle|\frac{\partial H}{\partial R^{\nu}}\middle|n\right\rangle-\left\langle n\middle|\frac{\partial H}{\partial R^{\nu}}\middle|n'\right\rangle\left\langle n'\middle|\frac{\partial H}{\partial R^{\mu}}\middle|n\right\rangle}{(\epsilon_n - \epsilon_n')^2}$$

```
(*Now we calculate the Berry curvature for this case*)
```

In[241]:=
```
MaTeX["\\Omega = i\\frac{\\left\\langle
n\\middle|\\frac{{\\partial}H}{{\\partial}q_x}\\middle|n'\\right\\rangle\\left\\
   langle
n'\\middle|\\frac{{\\partial}H}{{\\partial}q_y}\\middle|n\\right\\rangle-\\
   left\\langle
n\\middle|\\frac{{\\partial}H}{{\\partial}q_y}\\middle|n'\\right\\rangle\\left
   \\langle
n'\\middle|\\frac{{\\partial}H}{{\\partial}q_x}\\middle|n\\right\\rangle}{\\
   Delta^2 + 4q_x^2 + 4q_y^2\\tau_z^2}", Magnification → 1.5]
```

Out[241]=
$$\Omega = i\frac{\left\langle n\middle|\frac{\partial H}{\partial q_x}\middle|n'\right\rangle\left\langle n'\middle|\frac{\partial H}{\partial q_y}\middle|n\right\rangle-\left\langle n\middle|\frac{\partial H}{\partial q_y}\middle|n'\right\rangle\left\langle n'\middle|\frac{\partial H}{\partial q_x}\middle|n\right\rangle}{\Delta^2 + 4q_x^2 + 4q_y^2\tau_z^2}$$

In[243]:=
```
Ω = FullSimplify[((nBra.D[H, qx].npKet * npBra.D[H, qy].nKet) -
   (nBra.D[H, qy].npKet * npBra.D[H, qx].nKet)) * norm * i / δE^2]
```

Out[243]=
$$\left\{\left\{-\frac{2\,\Delta\,\tau_z}{\left(\Delta^2+4\,q_y^2+4\,q_x^2\,\tau_z^2\right)^{3/2}}\right\}\right\}$$

In[245]:=
```
Limit[Ω, Δ → 0] (* For gapless graphene. We expect a zero Berry curvature*)
```

Out[245]= {{0}}

In[246]:=
```
Export["Berry_Graphene.pdf", EvaluationNotebook[]]
```