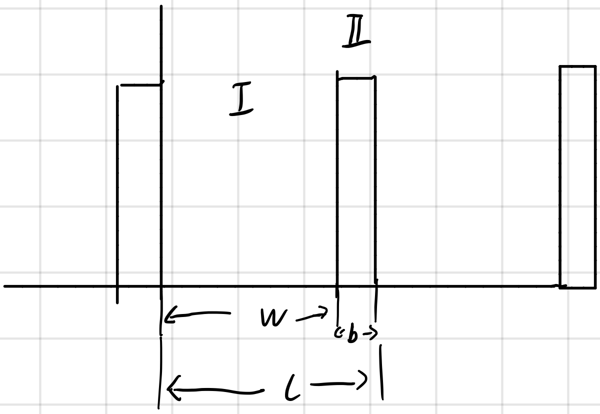
a)



for $E > V_1$

$$k_1 = \sqrt{\frac{2m_0}{\hbar^2}(E - V_0)}$$

$$k_3 = \sqrt{\frac{2m_0}{\hbar^2}(E - V_1)}$$

$$\psi_I = A e^{ik_1 x} + B^{-ik_1 x}$$

$$k_2 = \sqrt{\frac{2m_0}{\hbar}(V_1 - E)}$$

$$\psi_{II} = C e^{-ik_3 x} + D e^{ik_3 x}$$

$$k_2 = i k_3$$

$$\cos(kl) = \cos(k_1 w)\cosh(i k_3 b) + \frac{-k_3^2 - k_1^2}{2 i k_3 k_1} \sin(k_1 w)\sinh(i k_3 b)$$

$$\cosh(ik_3 b) = \cos(k_3 b)$$

$$\sinh(ik_3 b) = i\sin(k_3 b)$$

$$\Rightarrow \cos(kl) = \cos(k_1 w)\cos(k_3 b) - \frac{k_3^2 + k_1^2}{2k_3 k_1}\sin(k_1 w)\sin(k_3 b)$$

$$\frac{\hbar^2 k_1^2}{2m} = E - V_0 \qquad \frac{\hbar^2 k_2^2}{2m} = E - V_1$$

In[8]:= a = $\begin{pmatrix} \texttt{Exp[I k}_1\texttt{ w]} & \texttt{Exp[-I k}_1\texttt{ w]} & \texttt{-Exp[-I k}_2\texttt{ w]} & \texttt{-Exp[I k}_2\texttt{ w]} \\ \texttt{I k}_1\texttt{ Exp[I k}_1\texttt{ w]} & \texttt{-I k}_1\texttt{ Exp[-I k}_1\texttt{ w]} & \texttt{I k}_2\texttt{ Exp[-I k}_2\texttt{ w]} & \texttt{-I k}_2\texttt{ Exp[I k}_2\texttt{ w]} \\ \texttt{Exp[I kl]} & \texttt{Exp[I kl]} & \texttt{-Exp[-I k}_2\texttt{ l]} & \texttt{-Exp[I k}_2\texttt{ l]} \\ \texttt{I k}_1\texttt{ Exp[I kl]} & \texttt{-I k}_1\texttt{ Exp[I kl]} & \texttt{I k}_2\texttt{ Exp[-I k}_2\texttt{ l]} & \texttt{-I k}_2\texttt{ Exp[I k}_2\texttt{ l]} \end{pmatrix}$

Det[a]

Out[8]= $\{\{e^{i w k_1}, e^{-i w k_1}, -e^{-i w k_2}, -e^{i w k_2}\}, \{i e^{i w k_1} k_1, -i e^{-i w k_1} k_1, i e^{-i w k_2} k_2, -i e^{i w k_2} k_2\}, \{e^{i kl}, e^{i kl}, -e^{-i l k_2}, -e^{i l k_2}\}, \{i e^{i kl} k_1, -i e^{i kl} k_1, i e^{-i l k_2} k_2, -i e^{i l k_2} k_2\}\}$

Out[9]= $e^{i kl - i w k_1 + i l k_2 - i w k_2} k_1^2 - e^{i kl + i w k_1 + i l k_2 - i w k_2} k_1^2 - e^{i kl - i w k_1 - i l k_2 + i w k_2} k_1^2 + e^{i kl + i w k_1 - i l k_2 + i w k_2} k_1^2 + 4 k_1 k_2 + 4 e^{2 i kl} k_1 k_2 - 2 e^{i kl - i w k_1 + i l k_2 - i w k_2} k_1 k_2 - 2 e^{i kl + i w k_1 + i l k_2 - i w k_2} k_1 k_2 - 2 e^{i kl - i w k_1 - i l k_2 + i w k_2} k_1 k_2 - 2 e^{i kl + i w k_1 - i l k_2 + i w k_2} k_1 k_2 + e^{i kl - i w k_1 + i l k_2 - i w k_2} k_2^2 - e^{i kl + i w k_1 + i l k_2 - i w k_2} k_2^2 - e^{i kl - i w k_1 - i l k_2 + i w k_2} k_2^2 + e^{i kl + i w k_1 - i l k_2 + i w k_2} k_2^2$

In[10]:= **FullSimplify[%9]**

Out[10]= $4 e^{i kl} \left(\mathrm{Sin}[w k_1] \, \mathrm{Sin}[(l - w) k_2] \, k_1^2 + 2 \left(\mathrm{Cos}[kl] - \mathrm{Cos}[w k_1] \, \mathrm{Cos}[(l - w) k_2]\right) k_1 k_2 + \mathrm{Sin}[w k_1] \, \mathrm{Sin}[(l - w) k_2] \, k_2^2\right)$

$\mathrm{Det}(a) = 0 \, , \quad l - w = b$

$$(k_1^2 + k_2^2) \sin(k_1 w) \sin(k_2 b) + 2 k_1 k_2 \left(\cos(kl) - \cos(k_2 b) \cos(k_1 w)\right) = 0$$

$$\cos(kl) = \cos(k_1 w) \cos(k_2 b) - \frac{k_1^2 + k_2^2}{2 k_1 k_2} \sin(k_1 w) \sin(k_2 b)$$

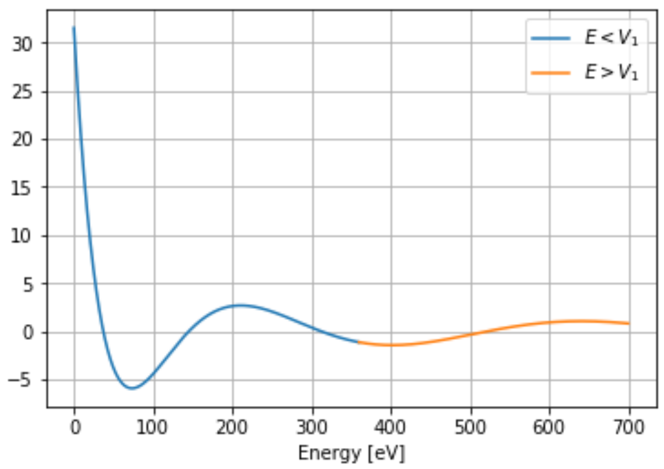
Q.E.D.

b)

In [40]:

```
import numpy as np
import matplotlib.pyplot as plt

m0 = 0.511e6     ## eV
c = 299792458   ##  m/s
hbar = 6.5821e-16    ##eV*s
ab = 5.29e-11       ##m
w = 1.5*ab
b = 0.5*ab

### E>V
def f0(E1, v0, v1):
    k1_0 = np.sqrt(2*m0*(E1-v0)/(hbar**2*c**2))
    k2_0 = np.sqrt(2*m0*(v1-E1)/(hbar**2*c**2))
    f0 = np.cos(k1_0*w)*np.cosh(k2_0*b) + (k2_0**2 - k1_0**2)/(2*k2_0*k1_0)*np.sin(k1_0*w)*np.
sinh(k2_0*b)
    return f0

### E<V
def f1(E2, V0, V1):
    k1_1 = np.sqrt(2*m0*(E2-v0)/(hbar**2*c**2))
    k2_1 = np.sqrt(2*m0*(E2-v1)/(hbar**2*c**2))
    f1 = np.cos(k1_1*w)*np.cos(k2_1*b) - (k2_1**2 + k1_1**2)/(2*k2_1*k1_1)*np.sin(k1_1*w)*np.s
in(k2_1*b)
    return f1

v0 = 0
v1 = 360
E1 = np.linspace(0.1, v1-0.1, 3600)
E2 = np.linspace(v1+0.1, 700, 3600)

f_0 = f0(E1, v0, v1)
f_1 = f1(E2, v0, v1)


plt.plot(E1, f_0, label = r'$E<V_1$')
plt.plot(E2, f_1, label = r'$E>V_1$')
plt.xlabel('Energy [eV]')
plt.grid()
plt.legend()
```

Out[40]: <matplotlib.legend.Legend at 0x7fe859519860>

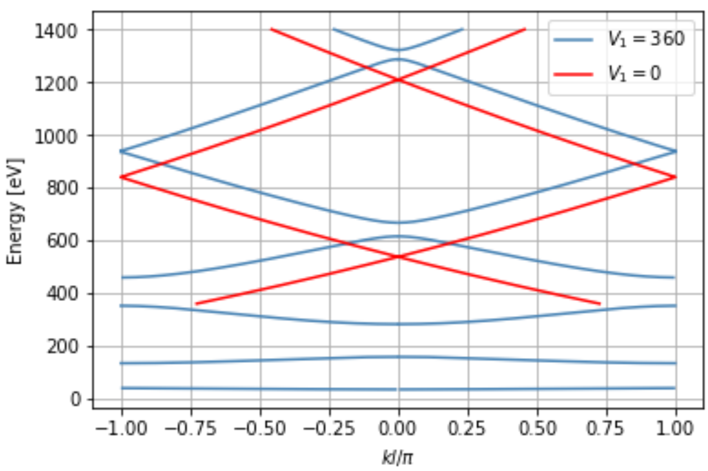


ci)

In [3]:
```
v0 = 0
v1 = 360
E1 = np.linspace(0.1, v1-0.1, 360000)
E2 = np.linspace(v1+0.1, 1400, 36000)

kl1 = np.arccos(f0(E1, v0, v1))/np.pi
kl2 = np.arccos(f1(E2, v0, v1))/np.pi

plt.plot( kl1 ,E1, c = 'steelblue')
plt.plot( -kl1 ,E1, c = 'steelblue')
plt.plot( kl2,E2, c = 'steelblue',  label = r'$V_1 =360$')
plt.plot( -kl2,E2, c = 'steelblue')
plt.ylabel('Energy [eV]')
plt.xlabel(r'$kl/\pi$')

v1 = 0.00001
kl100 = np.arccos(f0(E1, v0, v1))/np.pi
kl200 = np.arccos(f1(E2, v0, v1))/np.pi

plt.plot( kl100 ,E1, c = 'red')
plt.plot( -kl100 ,E1, c = 'red')
plt.plot( kl200, E2, c = 'red',  label = r'$V_1 =0$')
plt.plot( -kl200, E2, c = 'red')
plt.grid()
plt.legend()
```

```
/home/alex/.local/lib/python3.6/site-packages/ipykernel_launcher.py:6: RuntimeWarning: inval
id value encountered in arccos

/home/alex/.local/lib/python3.6/site-packages/ipykernel_launcher.py:7: RuntimeWarning: inval
id value encountered in arccos
  import sys
/home/alex/.local/lib/python3.6/site-packages/ipykernel_launcher.py:14: RuntimeWarning: inva
lid value encountered in sqrt
```

Out[3]: <matplotlib.legend.Legend at 0x7fe85ab014a8>

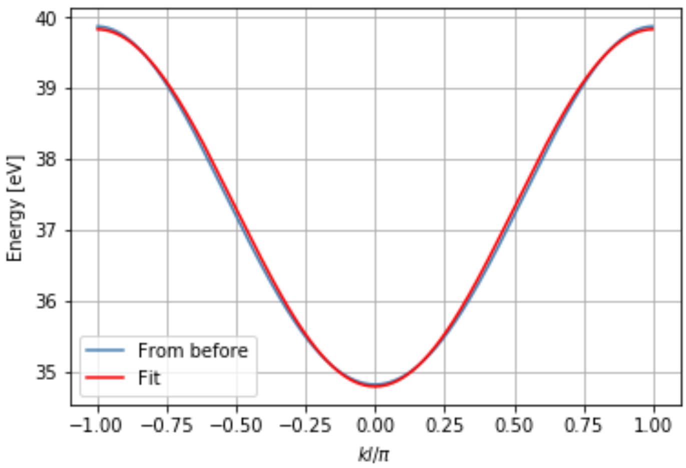


c i) The empty lattice represent forbiddent energies, where the energy is not allow in these range. This phenomenon can be found in semiconductor.

cii)

In [27]:
```
v1 = 360
v0 = 0
E = np.linspace(34, 40, 10000)
kl_low = np.arccos(f0(E, v0, v1))/np.pi

plt.plot(kl_low, E,c = 'steelblue',  label = 'From before')
plt.plot(-kl_low, E,c = 'steelblue')
plt.ylabel('Energy [eV]')
plt.xlabel(r'$kl/\pi$')


E0 = 37.31
t = 1.26
E_cos = E0 - 2*t*np.cos(kl_low*np.pi)
plt.plot(kl_low, E_cos, c = 'red', label = 'Fit')
plt.plot(-kl_low, E_cos, c = 'red')
plt.grid()
plt.legend()

E = np.append(-np.sort(-E[1365:9783]), E[1365:9783])
kl_low = np.sort(np.append(-kl_low[1365: 9783], kl_low[1365:9783]))
```

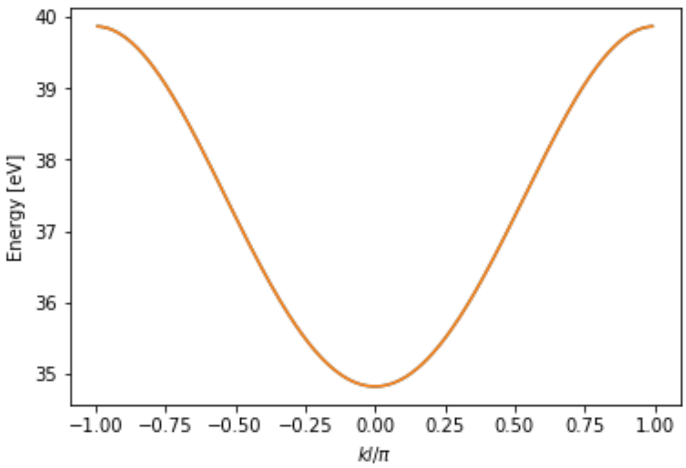
```
/home/alex/.local/lib/python3.6/site-packages/ipykernel_launcher.py:4: RuntimeWarning: inval
id value encountered in arccos
  after removing the cwd from sys.path.
```

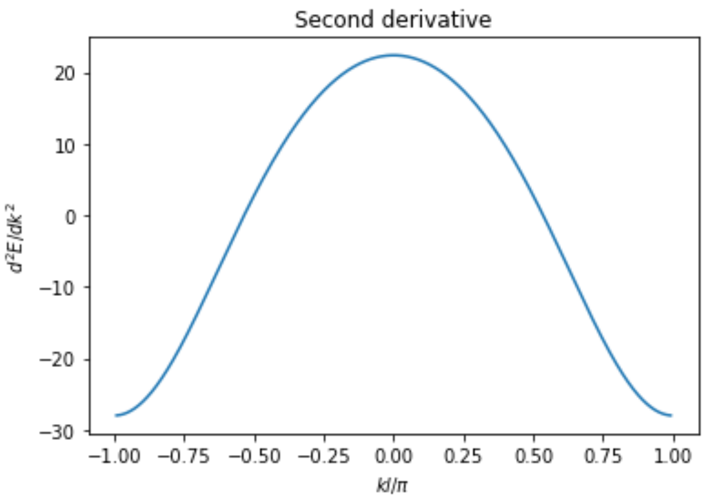


ciii)

In [30]:
```
from scipy.interpolate import UnivariateSpline


plt.figure()
plt.plot(kl_low, E)
E_sp = UnivariateSpline(kl_low,E,s=0,k=3)
plt.plot(kl_low, E_sp(kl_low))
plt.xlabel(r'$kl/\pi$')
plt.ylabel('Energy [eV]')
dE2_sp = E_sp.derivative(n = 2)
plt.figure()
plt.title('Second derivative')
plt.plot(kl_low, dE2_sp(kl_low))
plt.xlabel(r'$kl/\pi$')
plt.ylabel(r'$d^2E/dk^2$')
```

Out[30]:
```
Text(0,0.5,'$d^2E/dk^2$')
```





In [39]:
```
print('Second derivitive at 0: ',max(dE2_sp(kl_low)))
print('Second derivitive at k=pi/l: ',min(dE2_sp(kl_low)))

m_eff0 = hbar**2/max(dE2_sp(kl_low))
m_effp = hbar**2/min(dE2_sp(kl_low))

print('Electron:', m_eff0,' hole:', m_effp)
```

```
Second derivitive at 0:  22.371077015078793
Second derivitive at k=pi/l:  -27.98276817421869
Electron: 1.9366095061403733e-32  hole: -1.5482399789851975e-32
```

Since

$$\frac{d^2E}{dk^2} = \hbar^2/m_h^{eff}$$

and

$$\frac{d^2E}{dk^2} = \hbar^2/m_e^{eff}$$

So $m_{eff} = \hbar^2/\frac{d^2E}{dk^2}$.

As the result shows, the effective mass of the electrons are larger than the effective mass of the holes in magnitude. The curvature is smaller so the "hole" can move more freely.