HW 12

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2D electron gas system, 3D bulk material.
physical thickness

Quasi- 2D electron gas system: $E-(k_X,k_y)$,n : subband

We have calculated N_total : it is a scalar.
We want to calculate electron density. : n(x, y, z) It can generate $\phi(x,y,\ z)$

$N_{total}=\int n(x,y,z)dxdydz$

Required condition: $\int |\psi(x)|^2 dxdydz = 1$

Wave function : $\psi_{k_xk_yn}(x,y,z)=A_{k_xk_yn}e^{ik_xx}e^{ik_yy}\psi_{z,n}(z)$

: $\left|\psi_{k_xk_yn}(x,y,z)\right|^2=\left|A_{k_xk_yn}\right|^2\left|\psi_{z,n}(z)\right|^2$ thus Integration of $\left|\psi_{k_xk_yn}(x,y,z)\right|^2$ over the box :

$L_xL_y\left|A_{k_xk_yn}\right|^2\int_0^{L_z}dz\left|\psi_{z,n}(z)\right|^2 \ \ =1$ thus $\left|A_{k_xk_yn}\right|^2=\frac{1}{L_xL_y}$

Each state contributes $\left|\psi_{k_xk_yn}(x,y,z)\right|^2=\frac{\left|\psi_{z,n}(z)\right|^2}{L_xL_y}$

$n(x,y,z)=\sum_{n=1}^{\infty}\frac{|\psi|^2f_{FD}(E)}{L_xL_y}$

Schrodinger eqn discretization

: $-\frac{\hbar^2}{2m_{zz}}\frac{d^2}{dx^2}\psi_{z,n}(z)+V(z)\psi_{z,n}(z)=E_{z,n}\psi_{z,n}(z)$

-> $-\frac{\hbar^2}{2m_{zz}(\Delta z)^2}\left(\psi_{z,n,i+1}-2\psi_{z,n,i}+\psi_{z,n,i-1}\right)+(-q\phi(z)+E_c-E_i)\psi_{z,n,i}=E_{z,n}\psi_{z,n,i}$

$\int_0^{L_z}dz\left|\psi_{z,n}(z)\right|^2=1$

-> $\frac{\Delta z}{2}\left|\psi_{z,n,1}\right|^2=\frac{\Delta z}{2}\left|\psi_{z,n,N_z}\right|^2=0,\ \sum_{i=2}^{N_z-1}\Delta z\left|\psi_{z,n,i}\right|^2=1$

Simulation flow

$\phi(z)$
(semi-classical)

→

$\psi_{z,n}(z),E_{z,n}$
(with discretizated
Schrodinger eqn)

→

$n_{qm}(z)$
(use Poisson eqn
self-consistently)

We test six valleys in silicon which have two-fold degeneracy.

$$m_{xx} = 0.91m_0, m_{yy} = 0.19m_0, m_{zz} = 0.19m_0$$
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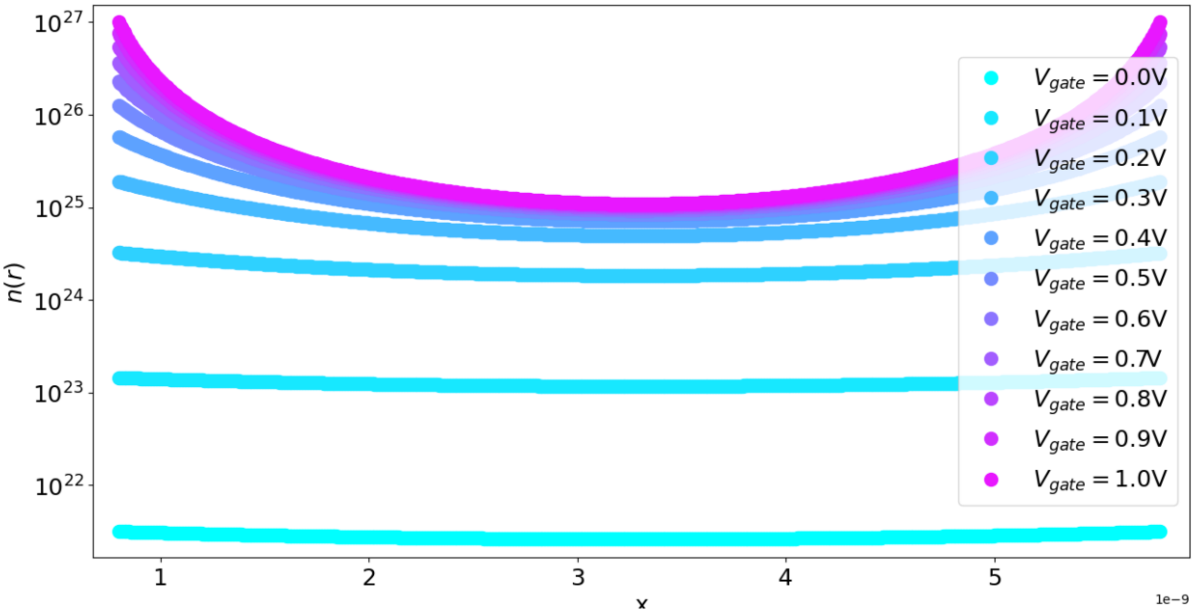
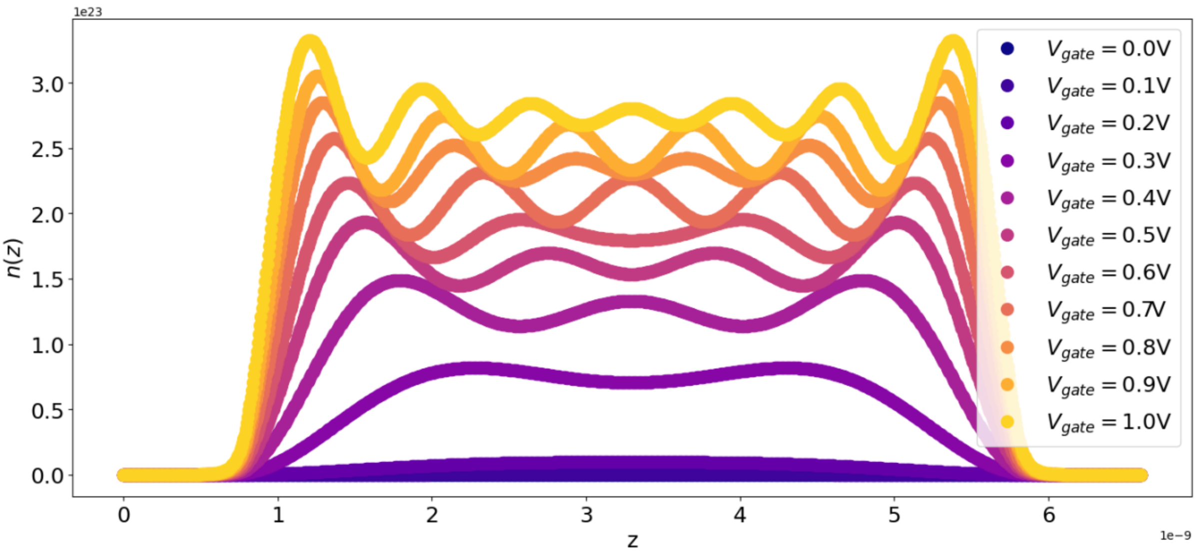
Result



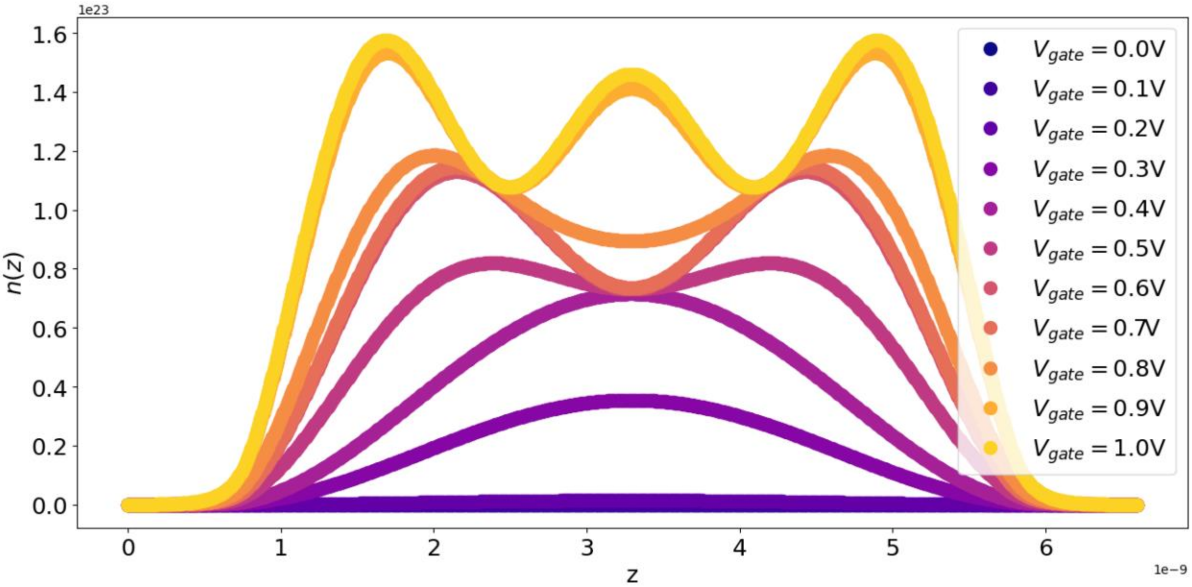
This figure shows the density with the semi-classical method.

1. $m_{zz} = 0.91m_0$(quantum mechanical result)



We now have wavy equations. Hight gate voltage makes more nodes in the density. We also find that maximum values of the density of quantum mechanical method is lower than that of semi-classical method at the same gate voltage.

2. $m_{zz} = 0.19m_0$ (quantum mechanical result)



Low effective mass of electrons shows similar forms of density with high effective mass of electron with low gate voltage.