HW 13

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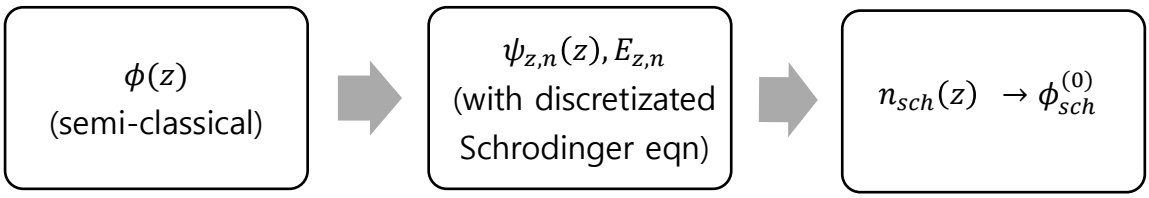
Simulation flow



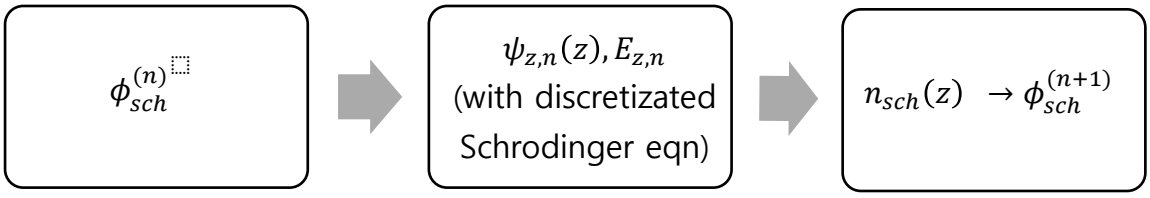
The first flow of the simulation is similar with hw12 before.

HW 12 : we set n_{sch} as constants. Thus we didn't use Newton-Raphson method. ϕ is earned newly with n_{sch}. And n_{sch} is earned newly with ϕ. ϕ and n_{sch} are updated self-consistently.

HW 13 : Now we set $n = n_{sch} * e^{\frac{\Delta\Phi}{V_T}}$. Therefore, we could use Newton-Raphson method as below. The first ϕ is semi-classically earned value.

$$residue = H\phi - \rho, (\rho = N_{acc} + n_{sch})$$
$$J = H - \frac{\partial\rho}{\partial\phi} = H - n_{sch}/V_T$$
$$J * \delta\phi = -\mathrm{r}$$
$$\rightarrow \phi^{(n+1)} = \phi^{(n)} + \delta\phi$$

Converged $\phi^{(n+1)}$ is now become the first quantum-mechanic-based value $\phi_{sch}^{(1)}$. We then use it to calculate the new ψ and n_{sch}.



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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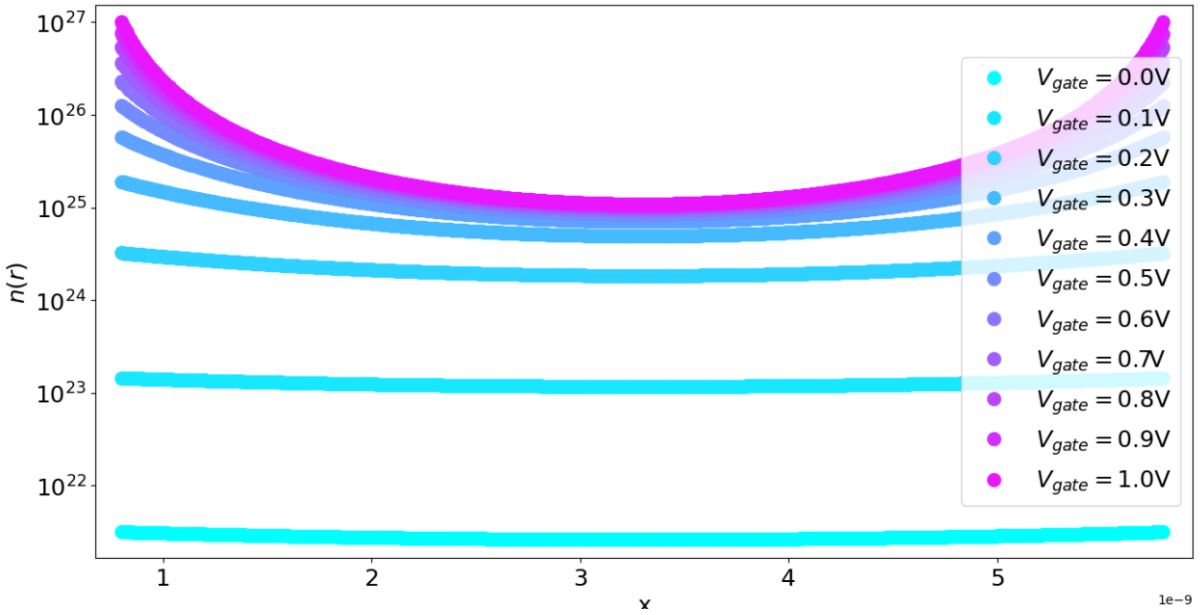
Convergence Criterion

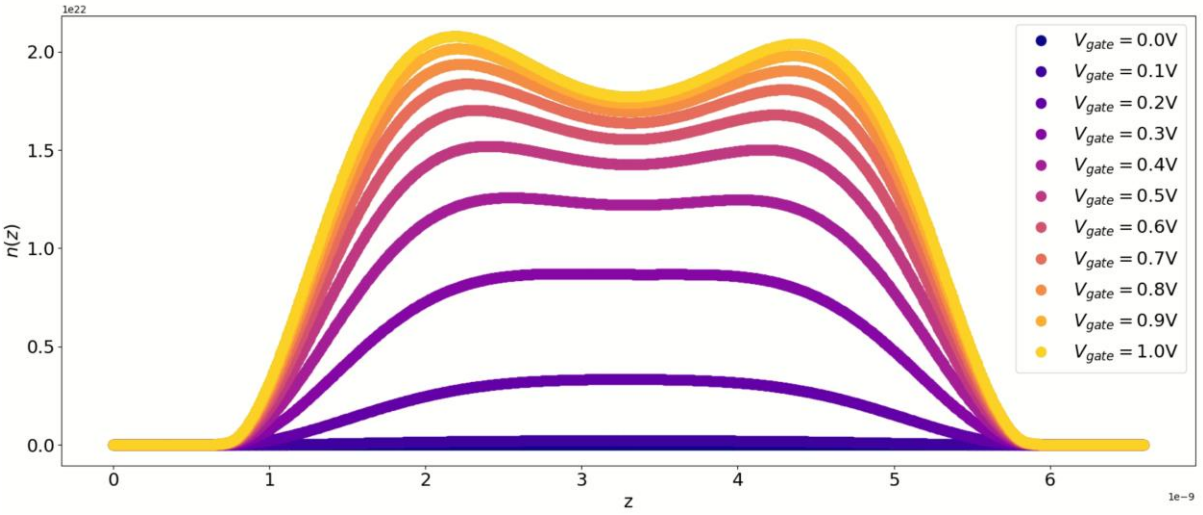
As the iteration goes, the fluctuation is largest around the center of $\phi(z)$. Thus, we finished iterations if it satisfies $\left|\phi^{(n)}(z = 3.3nm) - \phi^{(n-1)}(z = 3.3nm)\right| < 10^{-5}$.

Result



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

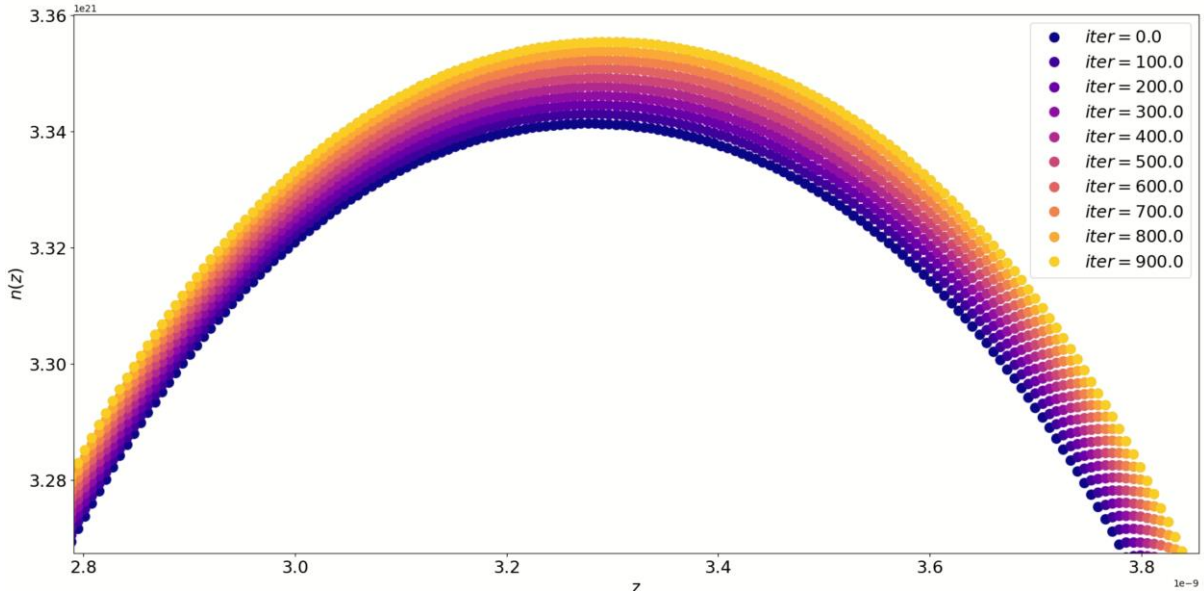
1. $m_{zz} = 0.91m_0$(quantum mechanical result)



We find that maximum values of the density of quantum mechanical method is lower than that of semi-classical method at the same gate voltage. It also looks like the form of the density is not symmetry with the high gate voltage.

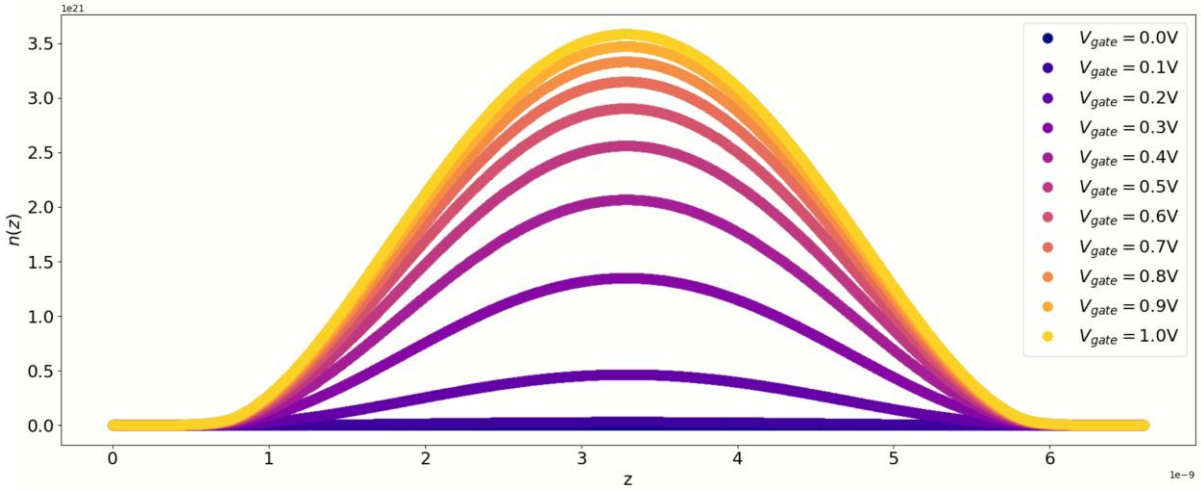
Every case (for any gate voltage) satisfies the convergence criterion. $\left|\phi^{(n)}(z = 3.3nm) - \phi^{(n-1)}(z = 3.3nm)\right| < 10^{-5}$. The final value at the gate voltage 0.2V : $\left|\phi^{(final)}(z = 3.3nm) - \phi^{(final-1)}(z = 3.3nm)\right| \simeq 10^{-8}$.

1.1 $V_{gate} = 0.2V$



We find that more iterations did not make smaller $\left|\phi^{(n)}(z = 3.3nm) - \phi^{(n-1)}(z = 3.3nm)\right|$ value. Upper figure shows the density with iterations. $\left|\phi^{(n)}(z = 3.3nm) - \phi^{(n-1)}(z = 3.3nm)\right| \simeq 10^{-8}$ But never converged.

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. The only difference is the maximum value of the density. More gate voltage makes higher maximum value of the density.