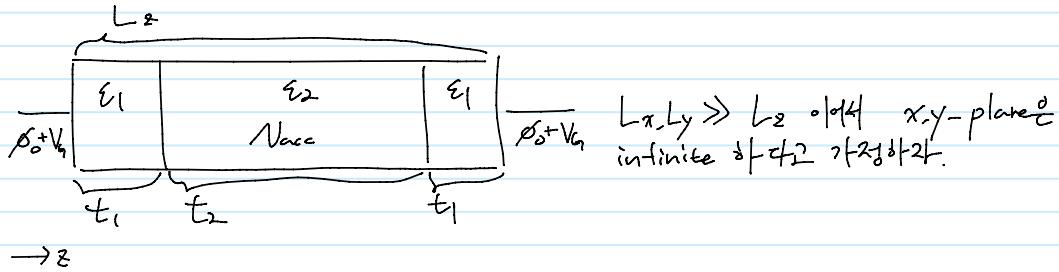


HW 12.

Thursday, October 15, 2020 5:01 PM

20184060 Jircheol Kim



$$\psi(x, y, z) = \frac{1}{L_{xy}} e^{ik_x x} e^{ik_y y} \sum_n \psi_n(z) \quad \text{where } \psi_n(z) \text{ is normalized.}$$

(Schrödinger eq.)

$$\left(-\frac{\hbar^2}{2m_{ee}} \frac{\partial^2}{\partial z^2} + V(z) \right) \psi_n(z) = E_n \psi_n(z)$$

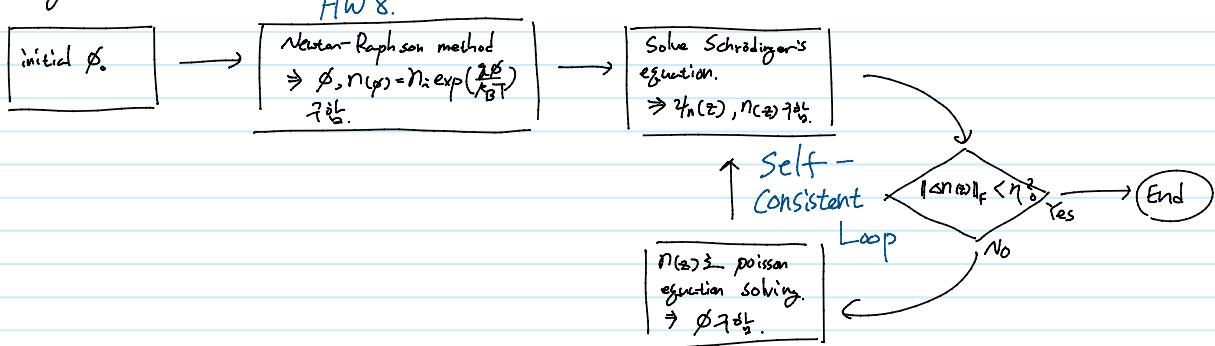
where $V(z) = -\phi(z) + (E_c - E_i)$ || $\phi(z)$ Poisson eq. $\frac{\partial}{\partial z} \phi(z) = -\frac{N(z)}{n(z)}$.

By discretization, numerically obtained $\psi_n^{(n)}$ takes a relation,

$$\sqrt{N-1} \psi_n^{(n)} = \sqrt{L_z} \psi_n(z). \quad \parallel \psi_n^{(n)} \rightarrow \sqrt{\frac{N-1}{L_z}} \psi_n^{(n)} \text{ or } \int_0^{L_z} \psi_n^{(n)} dz = 1 \text{ or } \frac{1}{\sqrt{N}}$$

$$\therefore N(z) = \frac{1}{L_{xy}} \sum_n |\psi_n(z)|^2 f(E_n) \quad \text{where } f(E) \text{ is Fermi-Dirac distribution.}$$

* Algorithm



Results.

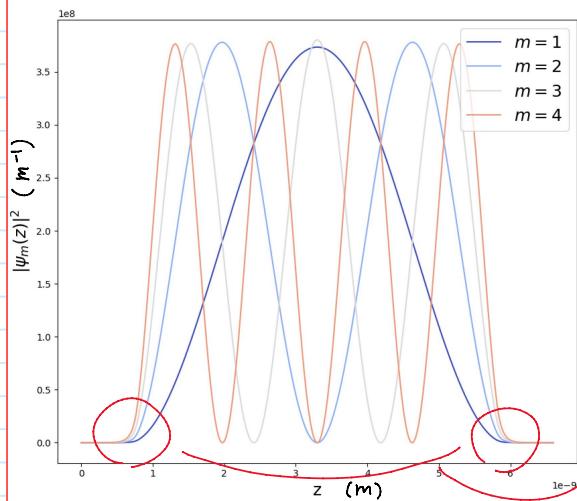
$$\phi_0 = 0.33374 \text{ V}, N = 800, N_{acc} = 10^{24} \text{ m}^{-3},$$

$$t_1 = 0.8 \text{ nm}, t_2 = 5 \text{ nm}, \epsilon_1 = 3.9 \epsilon_0, \epsilon_2 = 11.7 \epsilon_0,$$

$$E_c - E_i = \begin{cases} 0.56 \text{ eV} & \text{for Si, } E_F = 0 \text{ eV,} \\ 4.5 \text{ eV} & \text{for SiO}_2 \end{cases}$$

$$L_x = L_y = 100 \text{ nm}, m_{ee} \text{ of SiO}_2 = 0.58 m_e$$

(1) For $T = 300K$ with m_{zz} of $Si = 0.91 m_e$

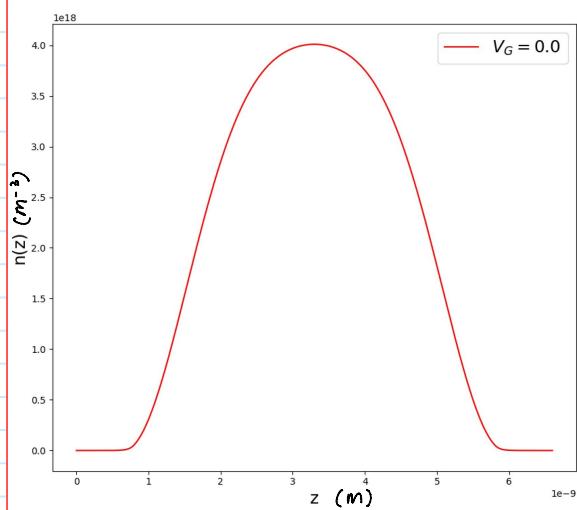


: Normalized $\psi_m(z)$ 으로 보면 $|\psi_m(z)|^2$.

SiO_2 의 band gap이 Si 보다 훨씬 크기 때문에

$\psi_m(z)$ 이 SiO_2 부문에서 exponentially decay 할 수 있다.

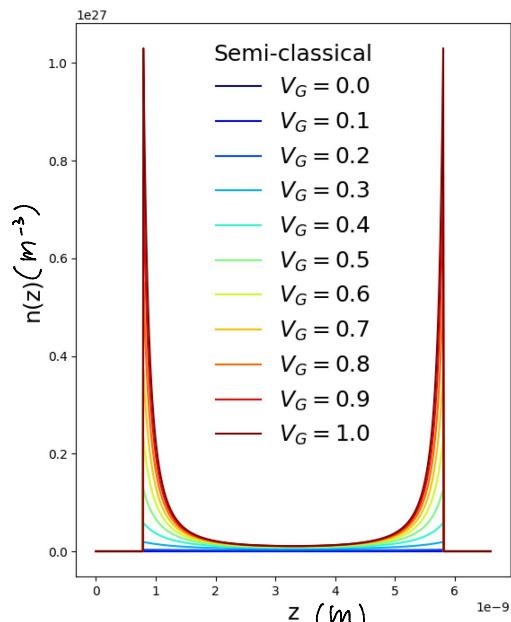
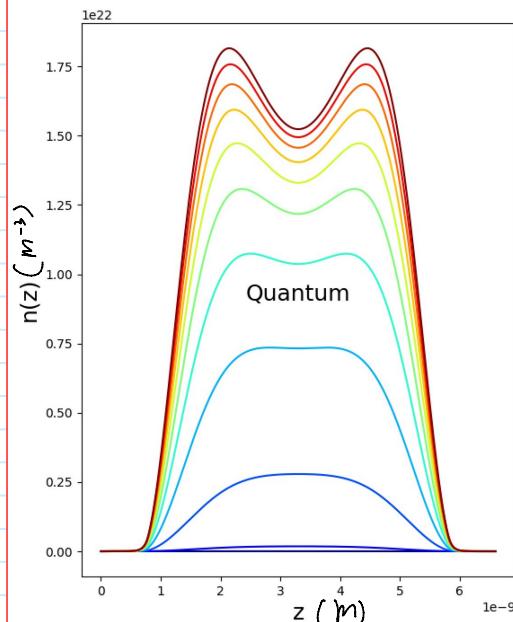
→ interface of tunneling 부분.



: electron density $n(z)$.

$f(E)$ 이 정하지 않으면, excited state와 ground state의 고려가 된다.

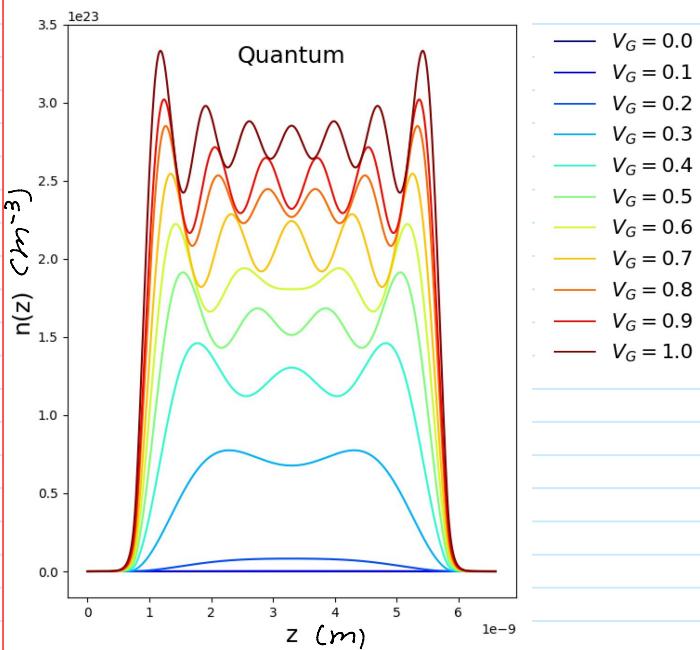
i) No self-consistent loop



: Quantum mechanical electron density vs Semi-classical electron density.

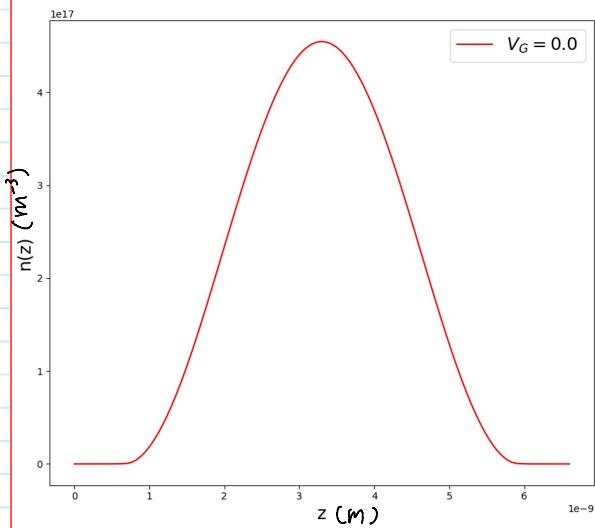
Scale부터 차이가 난다. quantum $n(z)$ 은 interface에서 peak가 생기질 않는다.

ii) Consider self-consistent loop



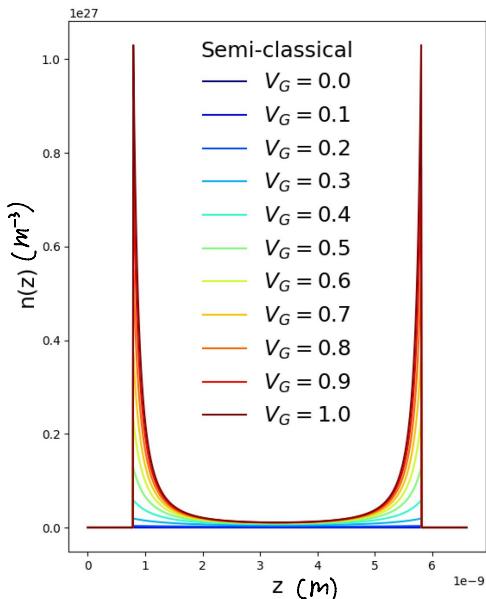
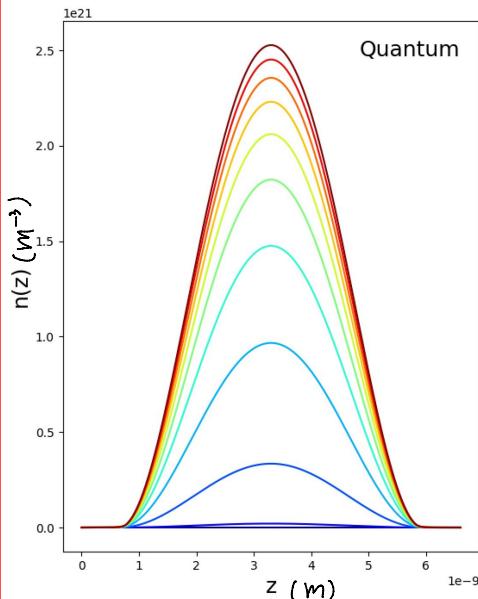
• Si 부분의 density는 wave function of interface에 exponentially decay 됨.
Gate voltage를 높일 수록 wave의 node가 많아짐.

(2) For $T = 300\text{K}$ with m_{zz} of Si = $0.19m_e$



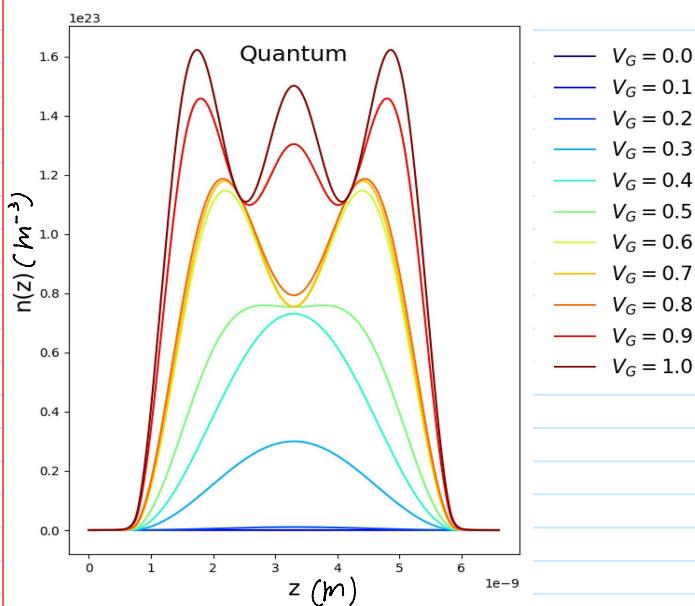
• $m_{zz} = 0.91m_e$ 일 때
 $n(z)$ 가 더 sharp해짐.

i) No self-consistent loop



• $m_{zz} = 0.91m_e$ 일 때
각각의 봉마다가 1/2
인 경우.

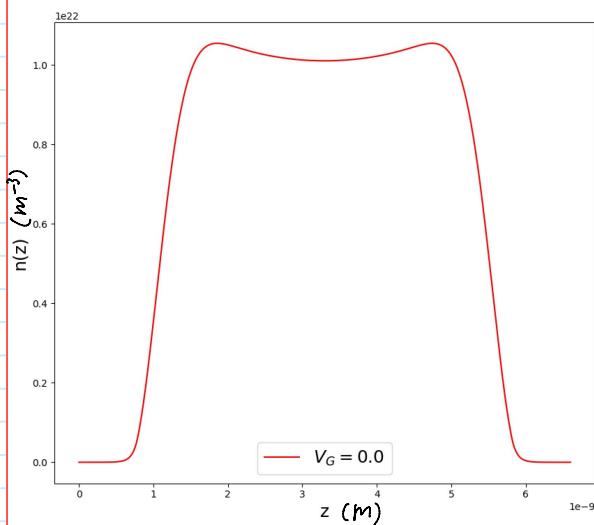
ii) Consider self-consistent loop



$\therefore M_{zz} = 0.91 m_e$ 를 cf. wave node?

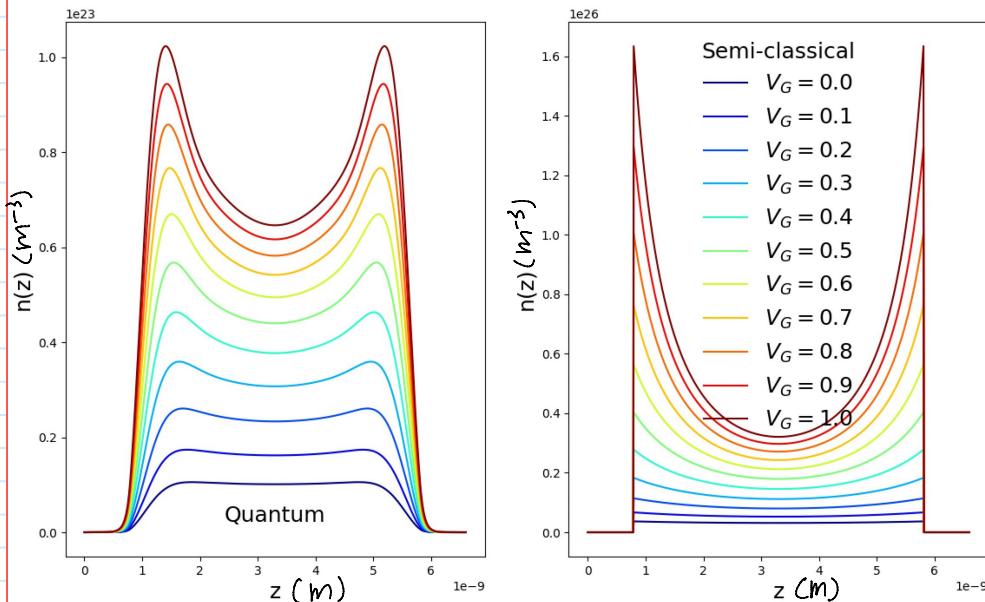
적다. Effective mass가 커져서呗, Energy level이 G 높아지 때문이다.

(3) For $T=1500\text{K}$ with M_{zz} of Si = $0.91 m_e$

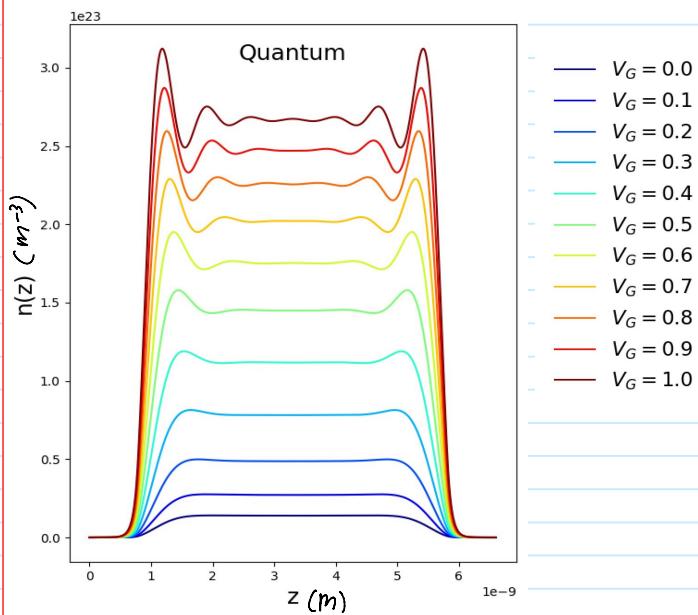


: Temperature가 높아서 $n(z)$ 이 미한 excited state의 기여가 $T=300\text{K}$ 보다 크다.
따라서, $n(z)$ 의 2주기 패턴이 보이진다.

i) No self-consistent loop

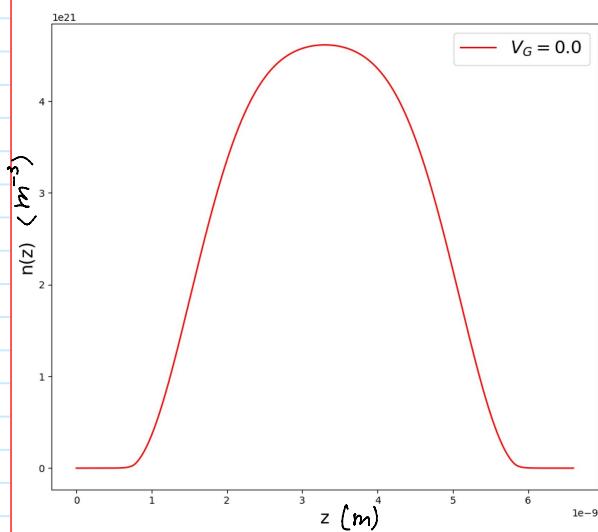


ii) Consider self-consistent loop



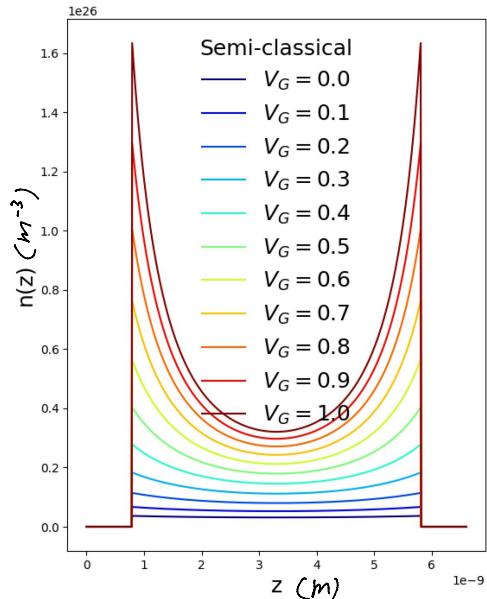
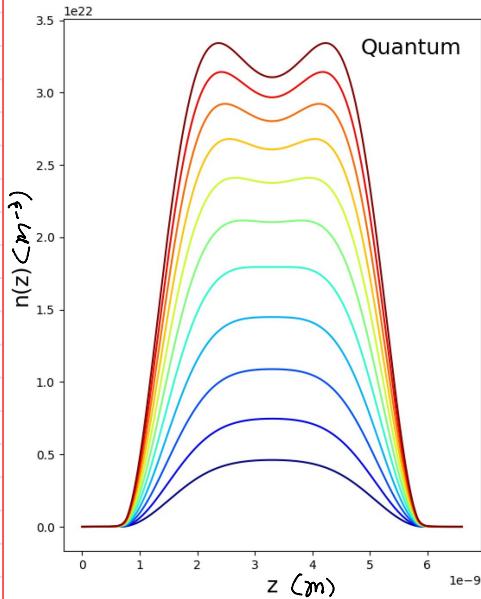
• Si 부분 density? $T=300\text{K}$ 이 10^23
이 flat state.
이는 high excited state들이 포함되어
Wave node가 불문명화되는 때이다.
high 한다.

(4) For $T=1500\text{K}$ with m_{zz} of Si = 0.19 m_e

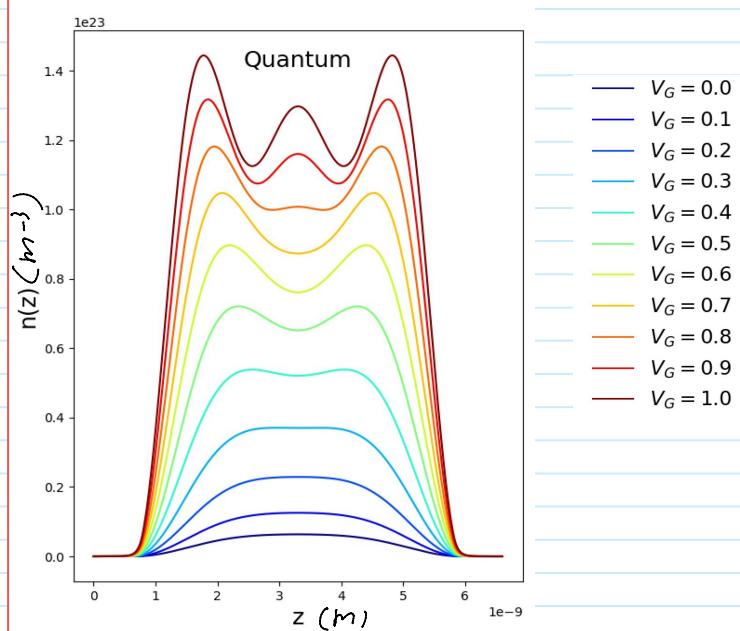


• $m_{zz} = 0.19m_e$ かつ $n(z)$?
sharp state.

i) No self-consistent loop



ii) Consider self-consistent loop



; of the high excited state
of the $T=300\text{K}$ case
wavy part is very flat
2D effect.