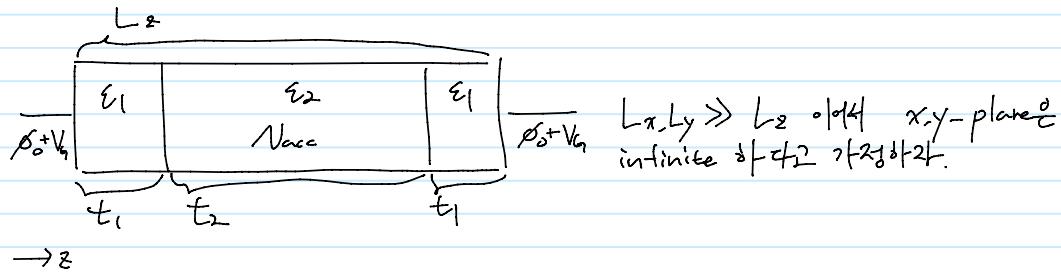


# HW 12.

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.)

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

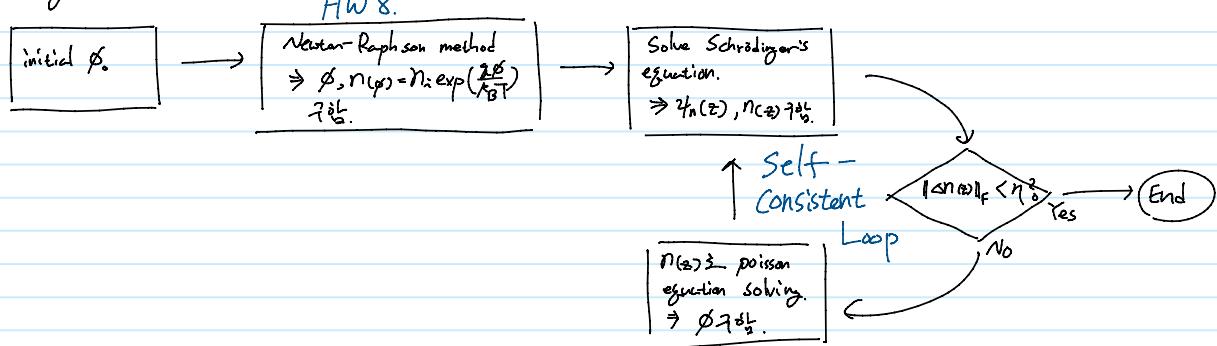
where  $V(z) = -\phi(z) + (E_c - E_i)$  ||  $\phi(z)$  Poisson eq.  $\frac{\partial}{\partial z} \phi(z) = -\frac{N(z)}{n(z)}$ .

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

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

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

\* Algorithm



Results.

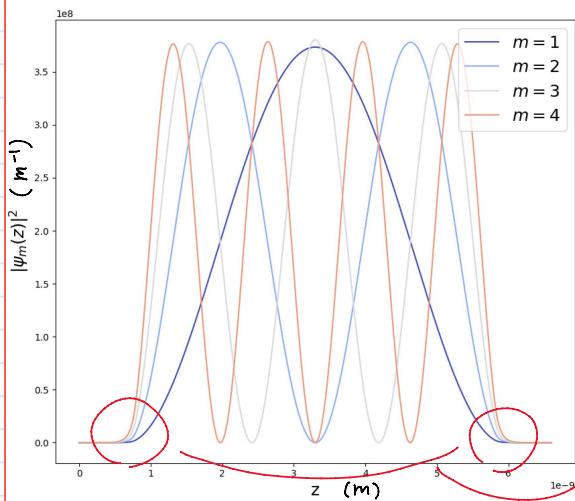
$$\phi_0 = 0.33374 \text{ V}, N = 800, N_{acc} = 10^{24} \text{ m}^{-3},$$

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

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

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

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

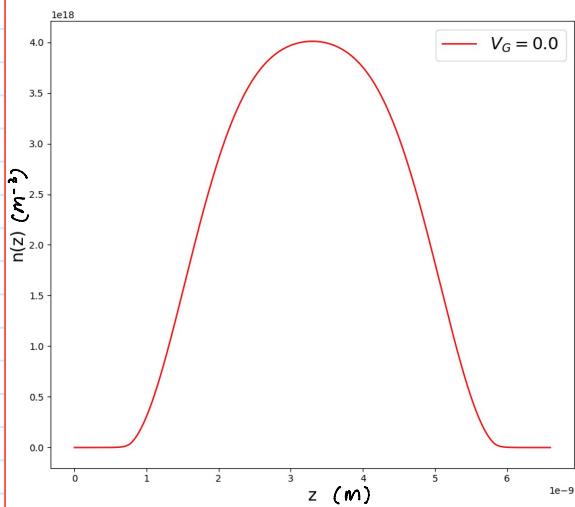


: Normalized  $\psi_m(z)$  으로 보면  $|ψ_m(z)|^2$ .

$SiO_2$ 의 band gap이  $Si$  보다 훨씬 크기 때문에

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

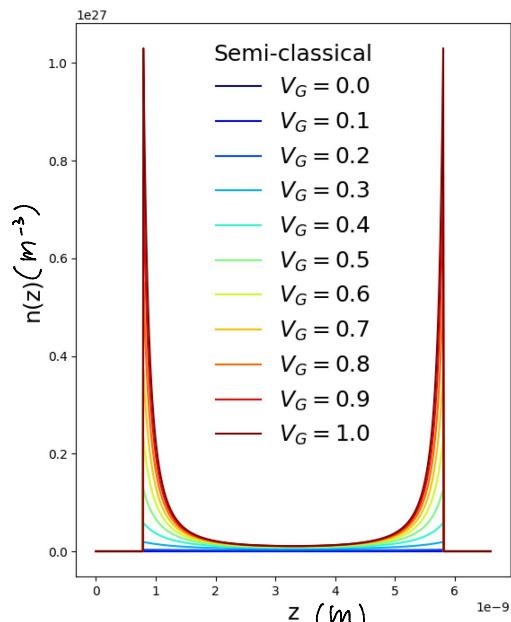
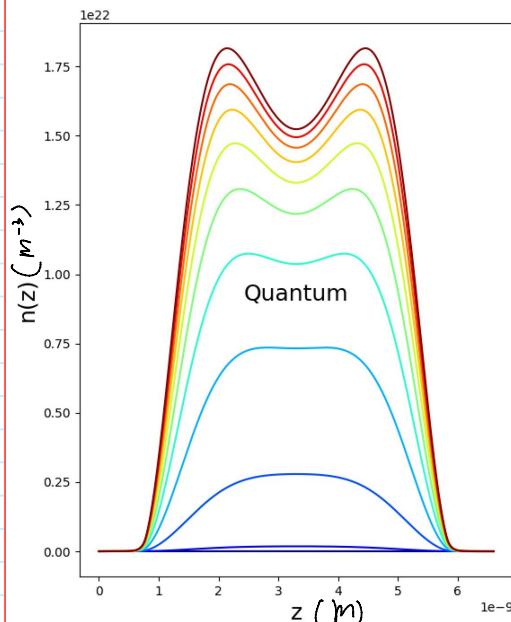
→ interface of tunneling 부분.



: electron density  $n(z)$ .

$f(E)$ 이 꽉 차지므로, excited state 및 ground state의 차이가 없다.

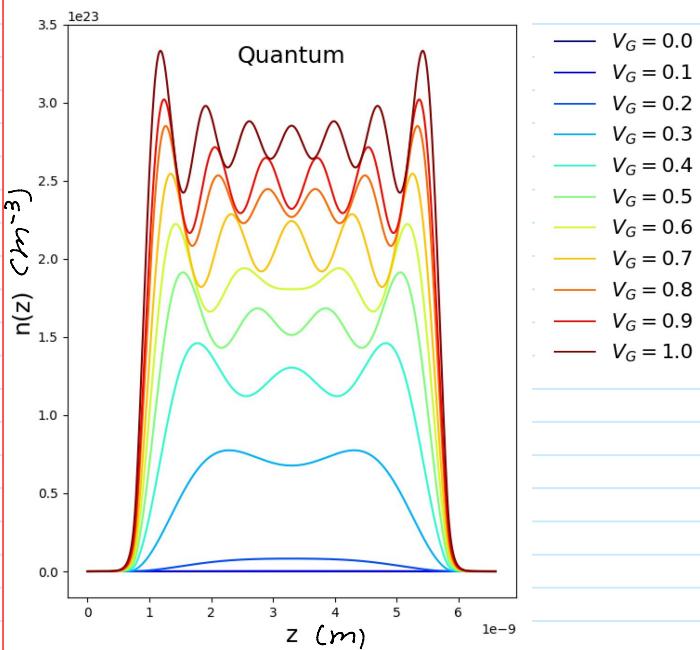
i) No self-consistent loop



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

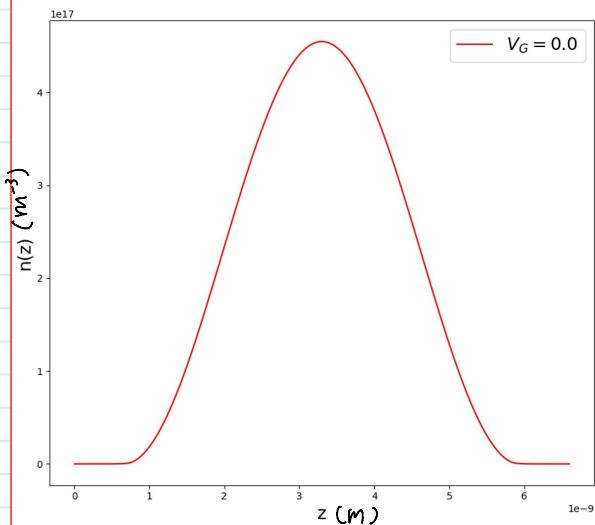
Scale부터 차이가 난다. quantum  $n(z)$ 은 interface에서 peak가 생기질 않는다.

ii) Consider self-consistent loop



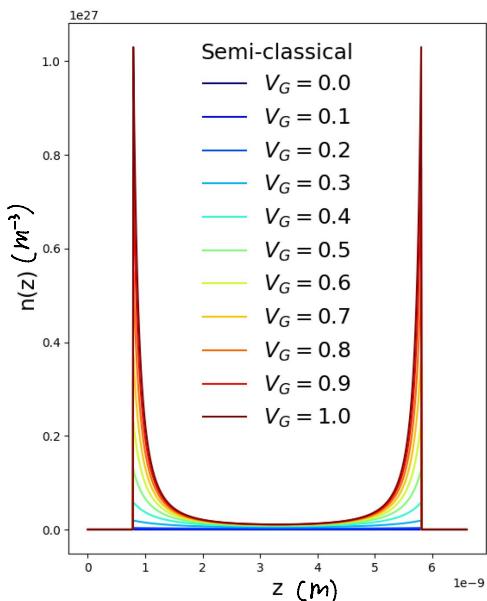
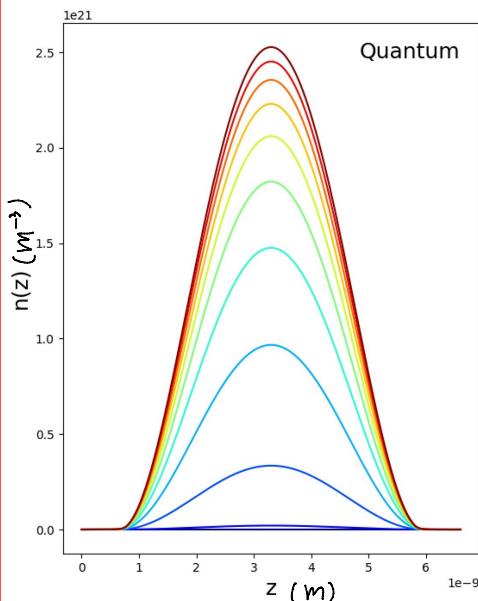
• Si 부분의 density는 wave function of interface에 exponentially decay 됨.  
Gate voltage를 높일 수록 wave의 node가 많아짐.

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



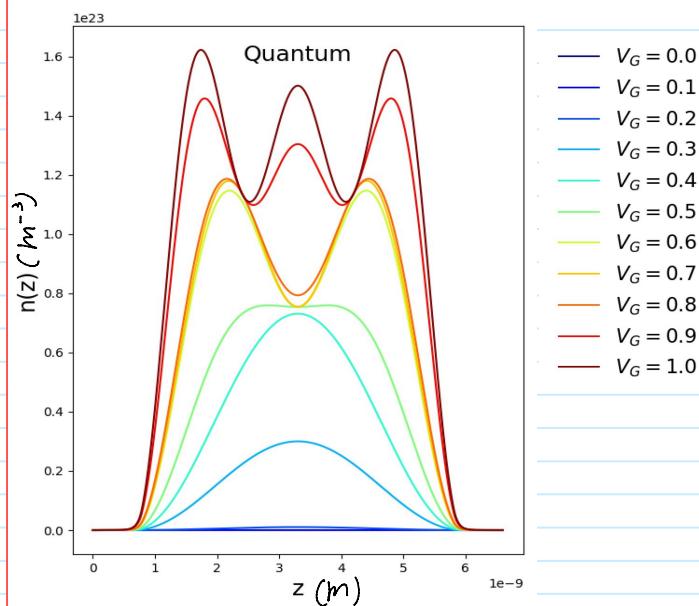
•  $m_{zz} = 0.19m_e$  일 때  
 $n(z)$ 가 더 sharp해짐.

i) No self-consistent loop



•  $m_{zz} = 0.19m_e$  일 때  
각각의 봉마다가 1/2  
인 경우.

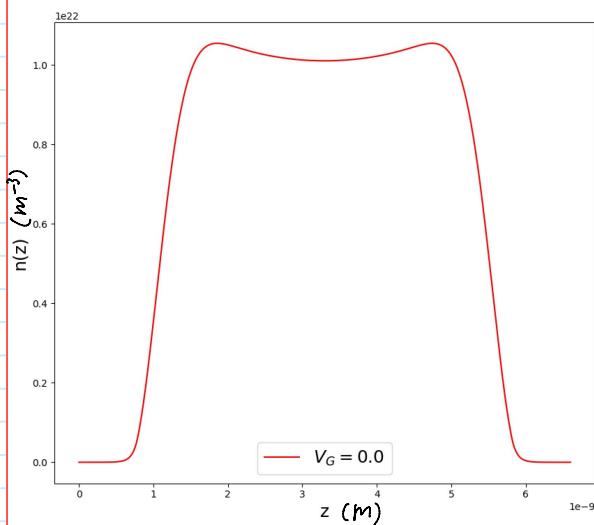
ii) Consider self-consistent loop



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

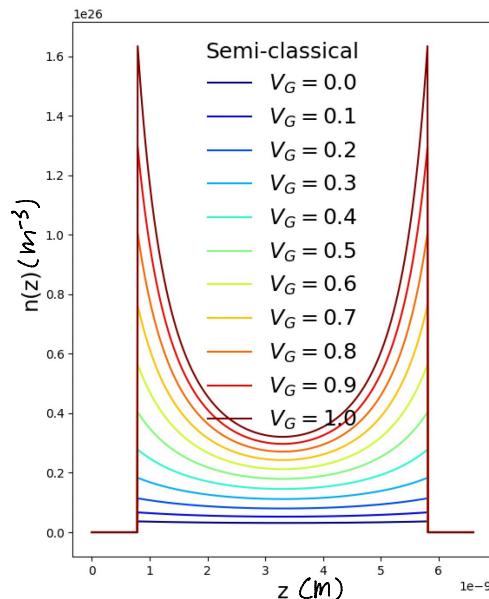
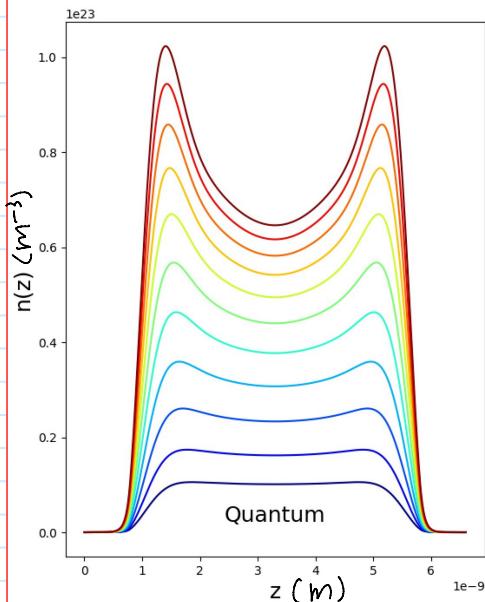
적다. Effective mass가 커져 있으니,  
Energy level이 G 높아지 때문이다.

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

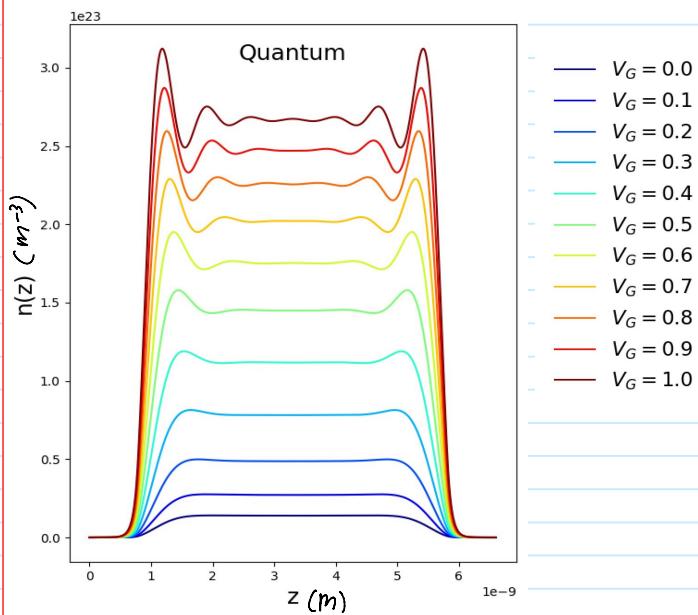


: Temperature가 높아서  $n(z)$ 이 미한  
excited state의 기여가  $T=300\text{K}$ 보다  
크다.  
따라서,  $n(z)$ 의 2주기 불규칙성이  
보이진다.

i) No self-consistent loop

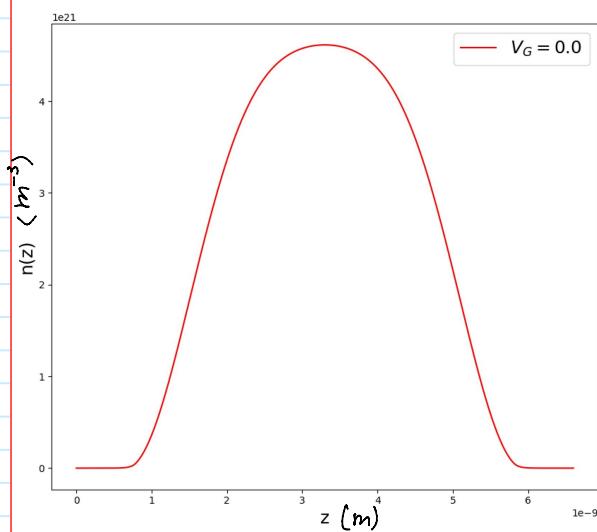


ii) Consider self-consistent loop



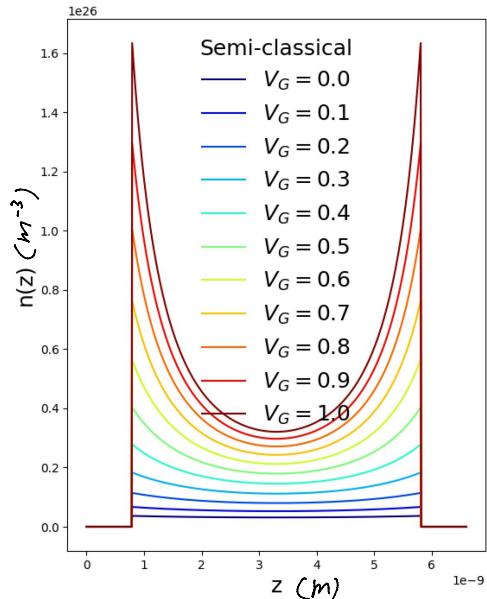
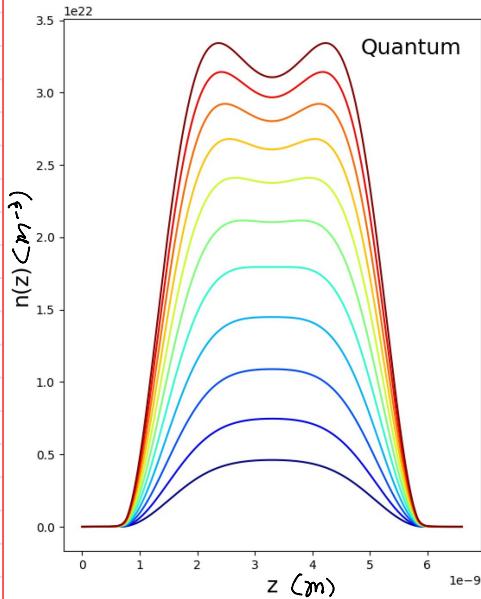
• Si 부분 density?  $T=300\text{K}$ 이 10^23  
이 flat state.  
이는 high excited state들이 포함되어  
Wave node가 불문명화되는 때이다.  
high 한다.

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

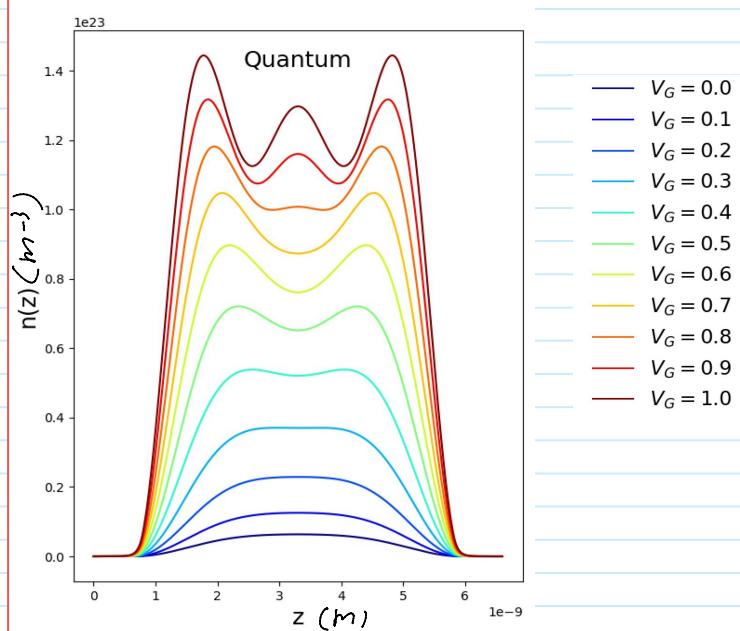


•  $m_{zz} = 0.19 m_e$ かつ  $n(z)$ ?  
sharp state.

i) No self-consistent loop



ii) Consider self-consistent loop



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