Project Q5.2

TCAD-based Simulation of Hole Spin Qubits in 5-Gate Si FinFETs: Rabi Frequency and Charge Noise

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Abstract - We performed TCAD simulations of Rabi frequency and electrostatic potential fluctuation at each qubit location, induced by single-charge traps. The simulation framework was applied to the 5-gate hole spin qubit Si FinFET fabricated at the University of Basel. Based on our formerly established AC simulation scheme, we developed post-processing code for the calculation of Rabi frequency. The simulated Rabi frequencies for the case of one-hole quantum dots (QDs) are ~ 480/29.8 GHz for QD1/2, which are orders of magnitude larger than the measured value (~ 20 MHz). This mismatch is likely due to a significant difference between the electrostatics of the real and simulated device. We simulate the potential fluctuation at each QD induced by displacement of single-charge traps - a useful prerequisite for the calculation of decoherence time and noise in future work. The obtained root mean square (*rms*) values of these potential fluctuations with just one single-charge interface trap in the whole device are ~ 4.9/4.6 mV at QD1/2, based on a set of 300 random trap locations. The device temperature is 1 K in all simulations.

Device Structure & Simulation Method

Device Structure:

- We studied the 5-gate Si FinFET fabricated at the University of Basel [1] (see Fig.1a), with two hole spin qubits embedded in QDs under the P-gates. Our goal is to establish a TCAD-based simulation framework capable of calculating the qubits' Rabi frequencies, the electrostatic potential and E-field fluctuation at each qubit location induced by single-charge traps. The simulated 3D device structure is shown in Fig.1b.

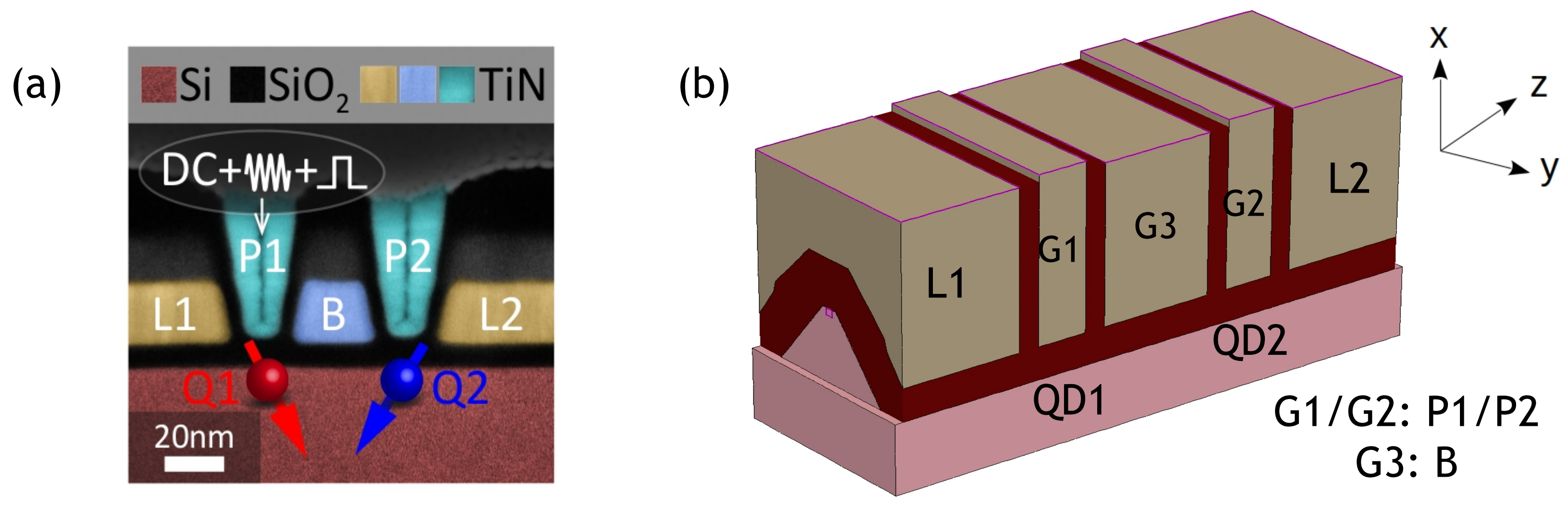
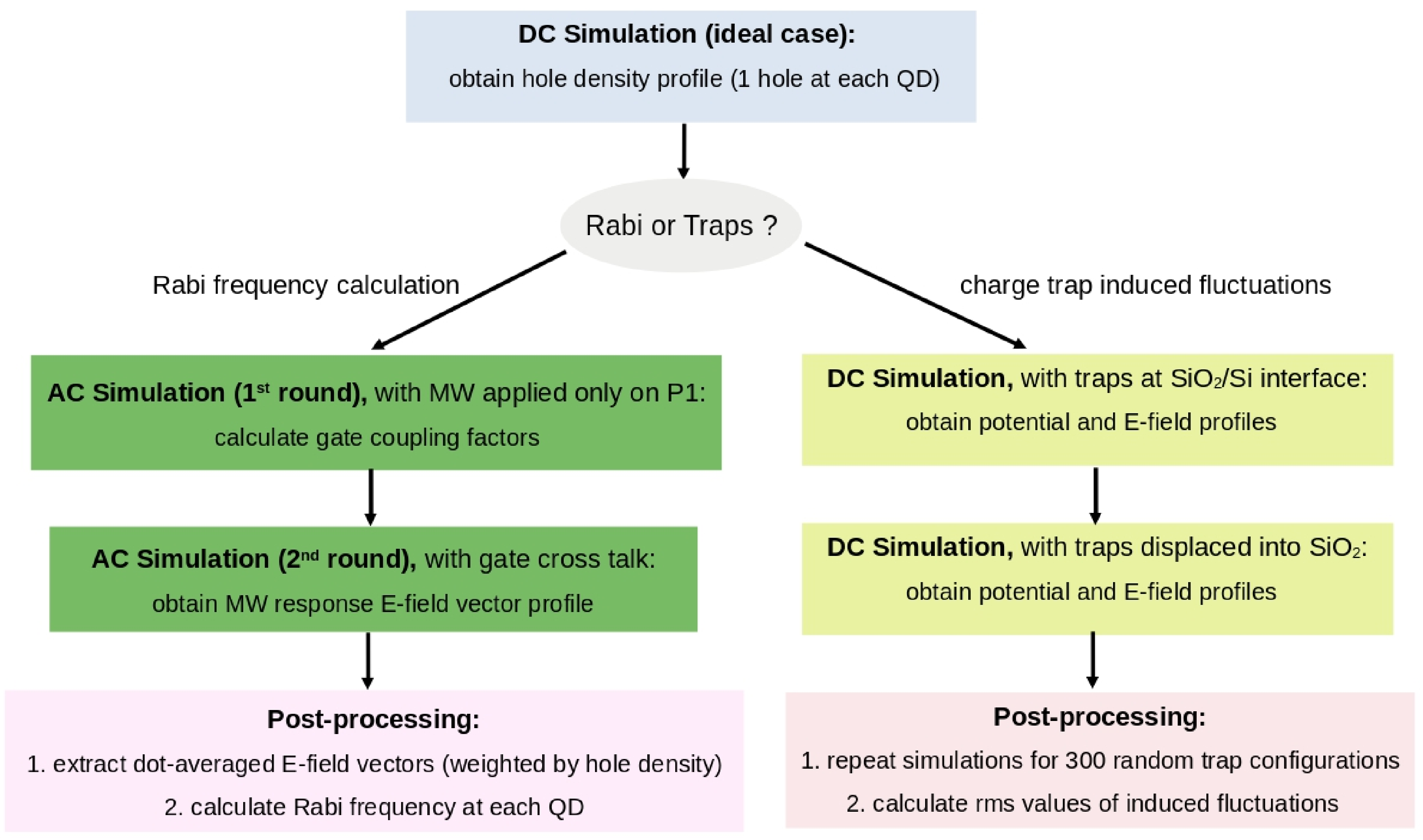


Figure 1: (a) 2D cross section of fabricated 5-gate Si FinFET device along fin direction, with double QDs formed under P-gates. (b). Sketch of simulated 3D device structure.

Simulation Method:

- Sentaurus Device is employed to solve for the electrostatics, with the density gradient model [2] used to capture the quantum confinement effect (calibrated with k·p Schrödinger-Poisson).
- The simulation flow is illustrated in Fig. 2.
  1) We implemented the theoretical model of Ref. [3] to calculate the Rabi frequency. One first runs a coupled DC-AC simulation to obtain the response E-field (amplitude and polarization angle) at each QD, then the self-developed post-processing code is used to obtain the Rabi frequency.
  2) For the trap-charge induced fluctuations, two-round DC simulations are performed: with charge traps directly at the gate SiO2/Si channel interface, and the traps displaced into SiO2 by 5 Å. From the change of potential caused by these trap displacements one calculates the correlation functions.



DC Simulation (ideal case):
obtain hole density profile (1 hole at each QD)

Rabi or Traps ?

Rabi frequency calculation

AC Simulation (1st round), with MW applied only on P1:
calculate gate coupling factors

AC Simulation (2nd round), with gate cross talk:
obtain MW response E-field vector profile

Post-processing:
1. extract dot-averaged E-field vectors (weighted by hole density)
2. calculate Rabi frequency at each QD

charge trap induced fluctuations

DC Simulation, with traps at SiO$_2$/Si interface:
obtain potential and E-field profiles

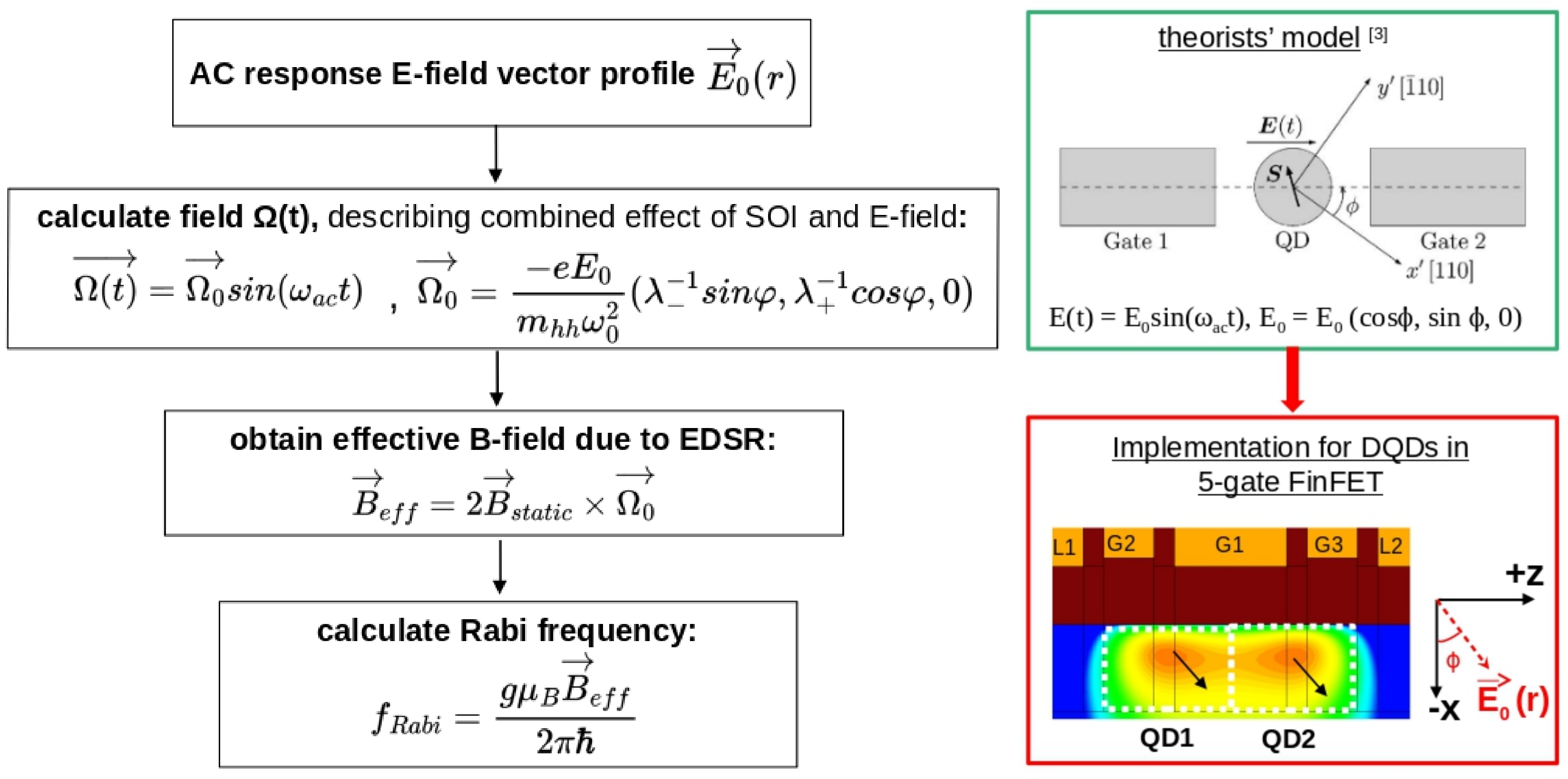
DC Simulation, with traps displaced into SiO$_2$:
obtain potential and E-field profiles

Post-processing:
1. repeat simulations for 300 random trap configurations
2. calculate rms values of induced fluctuations

Figure 2: Illustration of simulation flow for the calculation of Rabi frequency and electrostatic fluctuations induced by single-charge traps.

Simulation Results: Rabi Frequency

- Details of the post-processing code implemented for the studied device to calculate the Rabi frequency are described below.



AC response E-field vector profile $\vec{E}_0(r)$

calculate field Ω(t), describing combined effect of SOI and E-field:

$$\overrightarrow{\Omega(t)} = \vec{\Omega}_0 sin(\omega_{ac}t) \quad , \quad \vec{\Omega}_0 = \frac{-eE_0}{m_{hh}\omega_0^2}(\lambda_-^{-1}sin\varphi, \lambda_+^{-1}cos\varphi, 0)$$

obtain effective B-field due to EDSR:

$$\vec{B}_{eff} = 2\vec{B}_{static} \times \vec{\Omega}_0$$

calculate Rabi frequency:

$$f_{Rabi} = \frac{g\mu_B \vec{B}_{eff}}{2\pi\hbar}$$

theorists' model [3]

$E(t) = E_0 sin(\omega_{ac}t)$, $E_0 = E_0 (cos\phi, sin\ \phi, 0)$

Implementation for DQDs in 5-gate FinFET

- The obtained results of AC response E-field and Rabi frequency at QD1/2 (with one hole at each dot) are summarized in this table.

	ave. E_0 [V/cm]	Φ [˚]	B_{eff} [T]	f_{Rabi} [GHz]
QD1	4.62e5	17.65	(-16.87, 0, 5.36)	480.02
QD2	2.37e5	55.47	(-0.51, 0, 0.75)	29.79

Simulation Results: Trap-charge Induced Fluctuations

- The *rms* value of the trap-charge induced potential fluctuation averaged over each dot is calculated by the following formula:

$$\sqrt{\langle\delta V^2\rangle} = \frac{\int\int\int_{V_{QD}} \sqrt{\frac{\sum_{i=1}^{N}(V_i(r)-V'_i(r))^2}{N}}\, dr^3}{V_{QD}}$$

  - $V_i(r)$: potential profile with traps located directly at the SiO_2/Si interface
  - $V'_i(r)$: potential profile with traps vertically displaced into SiO_2 by 5 Å
  - N: total number of repeated simulation sets with randomly located single-charge traps
  - V_{QD} : volume of each single-hole QD
- The results for $\sqrt{\langle\delta V^2\rangle}$ based on 300 simulation sets (N=300) are summarized in the table below. The varied number of single-charge traps assigned in each simulation corresponds to the varied trap concentrations. δV is an abbreviation for $\sqrt{\langle\delta V^2\rangle}$.

# of single-charge traps	trap conc. [cm^{-2}]	QD1 δV [mV]	QD2 δV [mV]
1	1e11	4.86	4.61
7	1e12	18.74	19.69
36	5e12	43.44	43.66

- Assuming 1/f-noise, the trap-charge induced qubit dephasing time T_2^* can be calculated as follows[4]:

$$\frac{1}{T_2^*} = \frac{1}{\hbar}|\mathbf{Q}|\sqrt{\langle\delta V^2\rangle}\sqrt{\frac{1}{2\pi}\log\left(\frac{|\mathbf{Q}|\sqrt{\langle\delta V^2\rangle}}{\hbar\omega_{ir}}\right)}$$

Outlook

- Investigate impacts of the distance of trap displacement and DC hole charge configuration on the trap induced potential fluctuation
- Develop post-processing code to calculate single-charge trap induced qubit dephasing time T_2*

References

1. Camenzind et al., Nat Electron 5 (2022)
2. *Sentaurus* Device Manual, v2020.09
3. Golovachet al., Phys. Rev. B 74 (2006)
4. Bosco et al., PRX Quantum **2** (2021)