

# Device-Consistent Simulation of Spin Exchange Interaction in Quantum Dots Using Green's-Function Method for Inhomogeneous Dielectric Environments

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**Abstract**—We have developed a Green's-function-based method for computing the spin exchange interaction under an inhomogeneous dielectric environment, where the two-electron interaction cannot be described by the simple Coulomb form. Unlike conventional approaches assuming a homogeneous dielectric environment, the present method accurately treats structure-dependent two-electron interactions via electrostatic Green's-function solutions. This method enables device-consistent simulation of exchange interaction in quantum dot structures that exhibit dielectric inhomogeneity. Our simulations for Si double quantum dot structures reveal that dielectric inhomogeneity significantly affects the exchange interaction, highlighting the importance of the dielectric environment in Si spin qubit design.

**Index Terms**—Quantum computing, Quantum dots, Spin qubits

## I. INTRODUCTION

The large-scale integration of qubits is inevitably required to achieve the practical application of quantum computers. Silicon-based quantum computers, leveraging mature semiconductor fabrication technologies, are considered one of the most promising platforms for scalable quantum architectures. Si quantum computers are typically built on arrays of electron spins confined in quantum dots (QDs) electrostatically controlled by gate biases. Although various types of qubit-state encodings have been proposed [1], electrostatic control of the exchange interaction  $J_{\text{ex}}$  between electron spins plays a central role in qubit state manipulation. In particular, exchange-only qubits and their variants, which do not require microwave or external magnetic field and are suitable for large-scale integration, rely on precise control of  $J_{\text{ex}}$  [2], [3].

Recently, configuration interaction (CI) methods combined with Poisson-Schrödinger solvers have been developed to compute  $J_{\text{ex}}$  in realistic quantum device structures [4], [5]. In these approaches, single-electron wave functions are obtained in a manner consistent with the device geometry, while two-electron interaction is evaluated using a Coulomb kernel of the form  $e^2/(4\pi\kappa_{\text{Si}}\epsilon_0|r_1 - r_2|)$ , assuming a homogeneous

dielectric environment. Here,  $\kappa_{\text{Si}}$  is the dielectric constant of Si, and  $r_1, r_2$  are the coordinates of the electron. However, in a realistic device which has inhomogeneous dielectric environment, the potential  $V_G$  generated by an electron at  $r_2$  is generally given by the solution of the Poisson equation with position dependent dielectric constant  $\kappa(r)$  specific to the device structure,

$$\nabla_1 \cdot (\kappa(r_1)\epsilon_0 \nabla_1 V_G(r_1, r_2)) = -(-e)\delta(r_1 - r_2), \quad (1)$$

and therefore the interaction kernel itself is device-dependent. Consequently, achieving full consistency with the device structure requires incorporating the device-dependent interaction kernel into the two-electron integrals.

In this work, we present a CI-based framework in which all two-electron integrals are evaluated using electrostatic Green's-function (Poisson) solutions, enabling accurate treatment of dielectric inhomogeneity in QD devices. To the best of our knowledge, this is the first study that explicitly incorporates dielectric inhomogeneity into all two-electron integrals within a CI framework for quantum device simulations.

## II. METHOD AND MODEL

We consider a basic two-electron Hamiltonian for double QDs without external magnetic field,

$$H_{\text{DQD}} = \sum_p^{1,2} \left\{ -\frac{\hbar^2}{2m^*} \nabla_p^2 - eV_{\text{DQD}}(r_p) \right\} - eV_G(r_1, r_2), \quad (2)$$

where  $m^*$  is the effective mass, and  $V_{\text{DQD}}$  is the electrostatic potential experienced by an electron in the system. Firstly, single-electron orbitals  $\{\phi_i(r)\}$  ( $i = 1, \dots, N$ ) and  $V_{\text{DQD}}$  for the single-electron part corresponding to the first term in Eq. (2) are self-consistently obtained by 3D Poisson-Schrödinger simulations using our in-house TCAD simulator [6]–[8]. Based on these orbitals, we construct singlet and triplet basis sets as follows,

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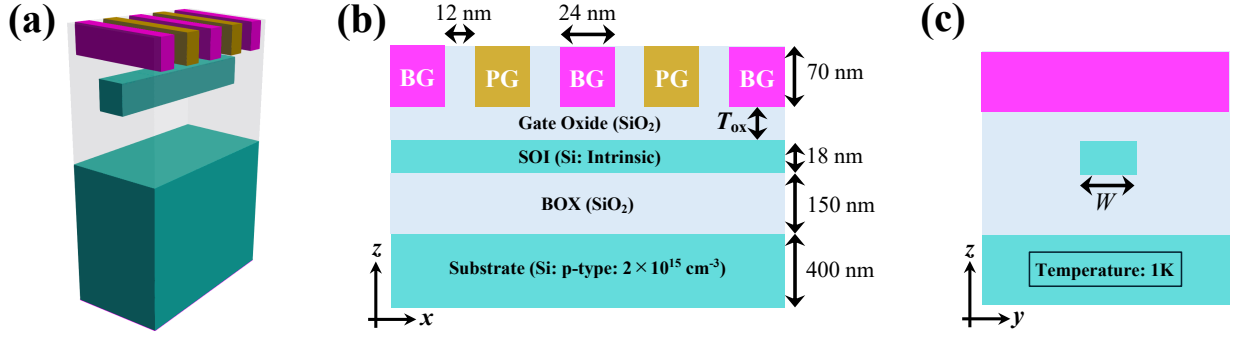


Fig. 1. (a) 3D schematic view of Si MOS-type double quantum dots with a Fin structure. (b),(c) 2D schematic view of Si MOS-type double quantum dots with a fin structure and its dimensions.

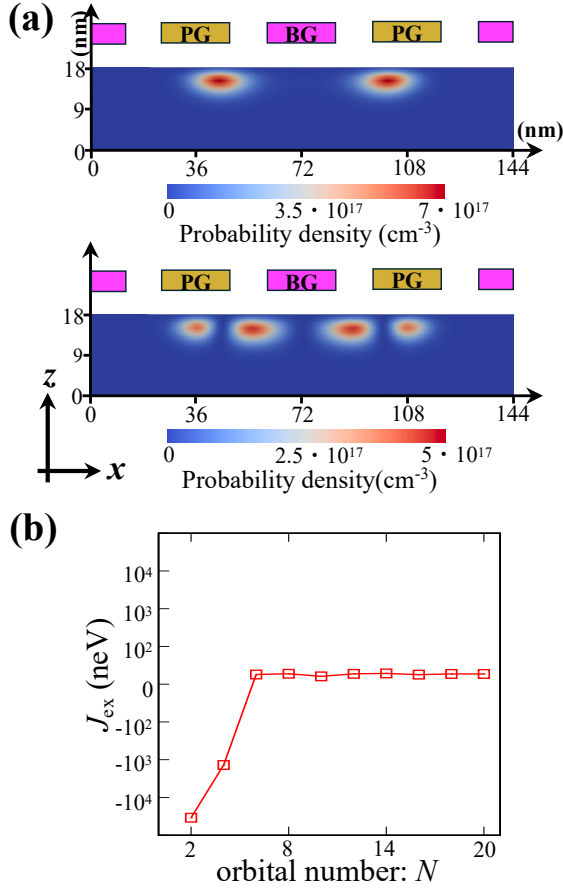


Fig. 2. (a) Representative spatial distributions of low-energy orbitals (ground and first excited states) in the  $x$ - $z$  plane. (b) Convergence of  $J_{\text{ex}}$  with respect to the number of orbitals  $N$ . A symmetric logarithmic scale is used, with a linear region around zero ( $|J_{\text{ex}}| < 100 \text{ neV}$ ).

$$\Psi_{i,j}^S = \begin{cases} \frac{1}{\sqrt{2}}(\phi_i(r_1)\phi_j(r_2) + \phi_i(r_2)\phi_j(r_1)) & (i \neq j), \\ \phi_i(r_1)\phi_j(r_2) & (i = j), \end{cases} \quad (3)$$

$$\Psi_{i,j}^T = \begin{cases} \frac{1}{\sqrt{2}}(\phi_i(r_1)\phi_j(r_2) - \phi_i(r_2)\phi_j(r_1)) & (i \neq j). \end{cases} \quad (4)$$

We then construct the singlet and triplet Hamiltonian matrices corresponding to Eq. (2). The matrix elements require

the evaluation of two-electron integrals of the following form,

$$\begin{aligned} \langle ij | -eV_G | kl \rangle &= -e \int \phi_i^*(r_1)\phi_j(r_1)V_G(r_1,r_2)\phi_k^*(r_2)\phi_l(r_2)dr_1dr_2 \\ &= -e \int \phi_i^*(r_1)\phi_j(r_1)\Phi_{kl}(r_1)dr_1, \end{aligned} \quad (5)$$

where  $\Phi_{kl}(r_1)$  is defined as follows,

$$\Phi_{kl}(r_1) = \int \phi_k^*(r_2)\phi_l(r_2)V_G(r_1,r_2)dr_2. \quad (6)$$

Since the analytical expression of  $V_G(r_1,r_2)$  is generally unavailable in an inhomogeneous dielectric environment, the integral in Eq. (5) cannot be evaluated directly. Instead of explicitly constructing the Green's function, we apply the differential operator  $\nabla_1 \cdot (\kappa(r_1)\epsilon_0\nabla_1)$  to Eq. (6) and, using Eq. (1), obtain the following Poisson equation for  $\Phi_{kl}(r_1)$ ,

$$\nabla_1 \cdot (\kappa(r_1)\epsilon_0\nabla_1\Phi_{kl}(r_1)) = -(-e)\phi_k^*(r_1)\phi_l(r_1), \quad (7)$$

which corresponds to the electrostatic potential generated by the fictitious charge density  $-e\phi_k^*\phi_l$ . Therefore, for every orbital products  $\phi_k^*\phi_l$ , we first solve Eq. (7) to obtain  $\Phi_{kl}$ , and then evaluate the two-electron integrals using the final expression in Eq. (5). In this manner, in contrast to the previous works which incorporate the device structure only at the single-electron level, our method extends the consistency with the device structure to the two-electron interaction kernel. Finally, the singlet and triplet Hamiltonians are diagonalized, and  $J_{\text{ex}}$  is obtained from the energy difference between their lowest-energy states.

As an application, we consider Si MOS-type double QDs with a fin structure (Fig. 1(a)) and evaluate the exchange interaction between electron spins. The basic device dimensions are shown in Figs. 1(b) and (c), and are chosen to reduce computational cost while preserving the essential physics governing exchange interaction. A Si (001) substrate is assumed. The confinement potential is formed by plunger gates (PGs) and barrier gates (BGs).  $J_{\text{ex}}$  is controlled by tuning the tunnel barrier via the voltage on the central barrier gate,  $V_{\text{BG}}$ . In this device structure, the electron wave functions are strongly confined along the  $z$ -axis, which is perpendicular to

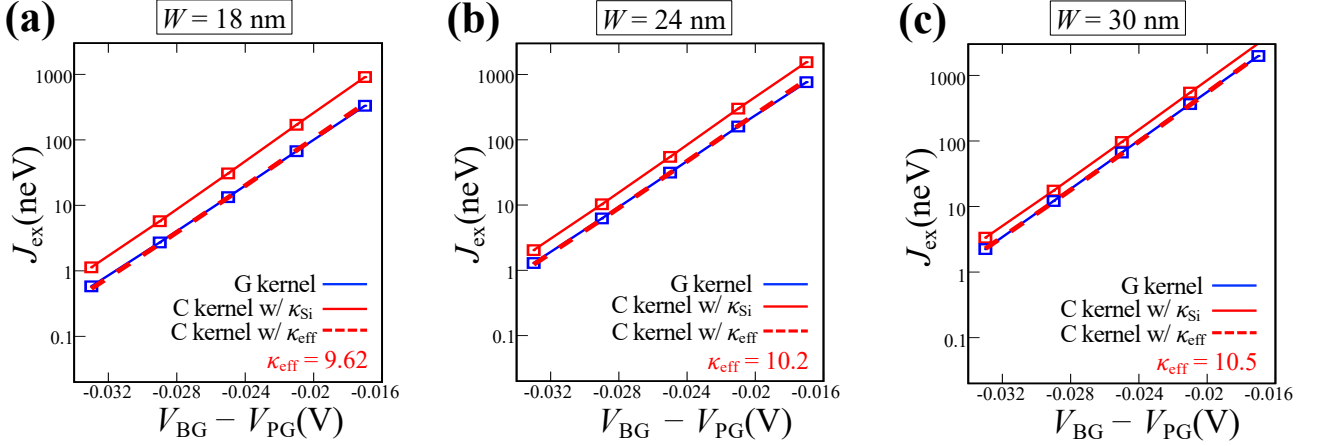


Fig. 3. (a)-(c)  $J_{\text{ex}}$  as a function of  $V_{\text{BG}} - V_{\text{PG}}$  for  $T_{\text{ox}} = 5$  nm and  $W = 18, 24, 30$  nm, respectively. Dashed lines represent the C-kernel with  $\kappa_{\text{eff}}$  calibrated to reproduce the G-kernel results.

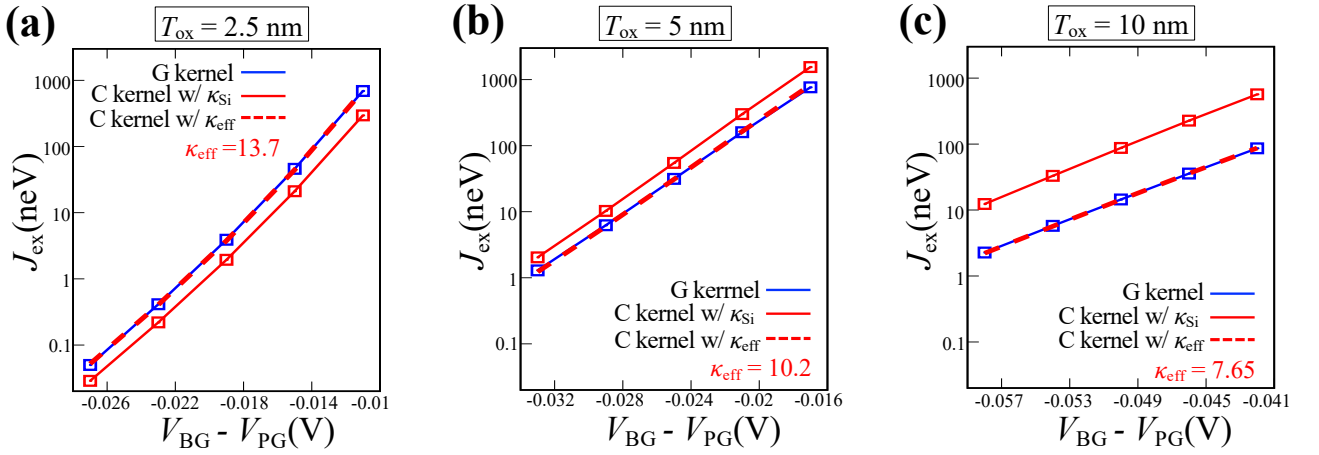


Fig. 4. (a)-(c)  $J_{\text{ex}}$  as a function of  $V_{\text{BG}} - V_{\text{PG}}$  for  $W = 24$  nm and  $T_{\text{ox}} = 2.5, 5, 10$  nm, respectively. Dashed lines represent the C-kernel with  $\kappa_{\text{eff}}$  calibrated to reproduce the G-kernel results.

the fin top plane. Therefore, only the low-energy ( $\Delta_2$ ) valley is considered within the effective-mass approximation. The longitudinal effective mass  $m_l = 0.98m_e$  is taken along the  $z$  direction, while the transverse effective mass  $m_t = 0.19m_e$  is used along the  $x$  and  $y$  direction. Figure 2 (a) shows the examples of spatial distributions of low-energy orbitals for the device structure in the  $x$ - $z$  plane with  $T_{\text{ox}} = 5$  nm and  $W = 24$  nm, demonstrating that the orbitals are localized near the fin top. The dependence of  $J_{\text{ex}}$  on the number of orbital  $N$  is also examined. Figure 2 (b) is the calculated  $J_{\text{ex}}$  as a function of  $N$  for a representative device structure and bias condition.  $J_{\text{ex}}$  is well converged at  $N = 20$ , ensuring the reliability of the CI calculated results. All results presented in this work are obtained using  $N = 20$ . We investigate the dependence of  $J_{\text{ex}}$  on the fin width  $W$  and the oxide thickness  $T_{\text{ox}}$ , which modify the electrostatic environment surrounding the quantum dots.

### III. RESULTS AND DISCUSSION

We first determine the gate voltages where the ground-state energies of both quantum dots align with the Fermi level, and then evaluate  $J_{\text{ex}}$  as a function of  $V_{\text{BG}}$ . Figures 3 (a)-(c)

show  $J_{\text{ex}}$  for fixed oxide thickness  $T_{\text{ox}} = 5$  nm and  $W = 18, 24, 30$  nm. Here, the horizontal axis represents  $V_{\text{BG}}$  relative to the plunger gate voltage  $V_{\text{PG}}$ . The red and blue curves indicate calculations using a homogenous Coulomb kernel with  $\kappa_{\text{Si}} = 11.7$  (C-kernel with  $\kappa_{\text{Si}}$ ) and our inhomogeneous Green's-function-based kernel (G-kernel), respectively. For the C-kernel calculations, we employ a Fourier-space approach based on truncated Coulomb potentials [9]. The calculated dependence of  $J_{\text{ex}}$  on gate voltage exhibits an exponential behavior consistent with experimentally observed trends [10]. These figures show that the C-kernel with  $\kappa_{\text{Si}}$  leads to a systematic misestimation of  $J_{\text{ex}}$  due to electric field leakage into surrounding regions. As  $W$  increases, the discrepancy between the C-kernel and the G-kernel results becomes smaller. To interpret this trend, we introduce an effective dielectric constant  $\kappa_{\text{eff}}$ , calibrated such that the C-kernel reproduces the G-kernel results. The dashed red curves indicate the results using this calibrated  $\kappa_{\text{eff}}$ . The resulting  $\kappa_{\text{eff}}$  approaches  $\kappa_{\text{Si}}$  as  $W$  increases, reflecting increased confinement of the electric field within the Si region.

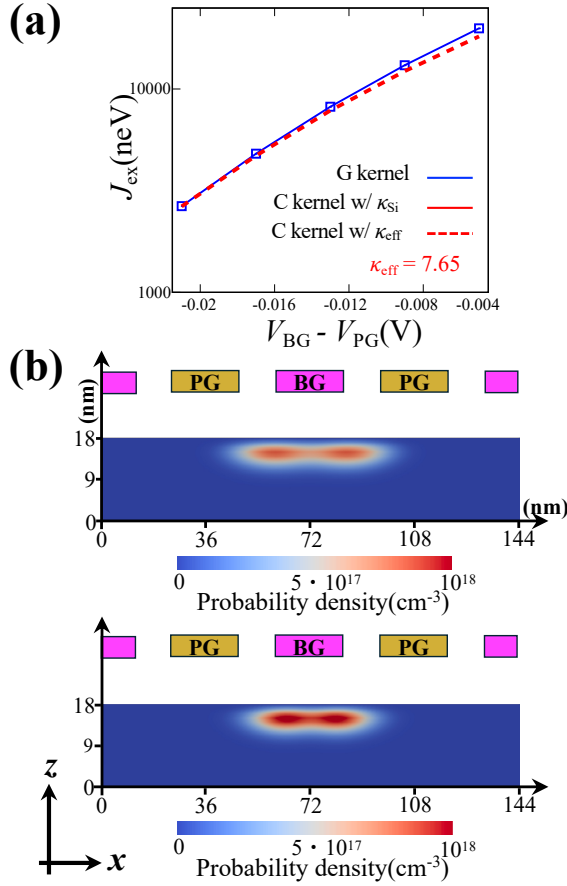


Fig. 5. (a)  $J_{\text{ex}}$  as a function  $V_{\text{BG}} - V_{\text{PG}}$  for  $W = 24$  nm and  $T_{\text{ox}} = 10$  nm under high  $V_{\text{BG}}$  condition. A dashed line represents the C-kernel with  $\kappa_{\text{eff}}$ . (b) Summed electron probability density of the ground-state orbital pair for  $V_{\text{BG}} - V_{\text{PG}} = -0.02$  V (top) and  $-0.004$  V (bottom), respectively.

Next, figures 4(a)-(c) show  $J_{\text{ex}}$  for fin width  $W = 24$  nm and  $T_{\text{ox}} = 2.5, 5, 10$  nm. Thinner oxide thickness enhances the electrostatic control of the barrier gate, leading to a stronger modulation of the tunnel barrier between the dots. Hence, the dependence of  $J_{\text{ex}}$  on  $V_{\text{BG}}$  becomes stronger as  $T_{\text{ox}}$  decreases. Increasing  $T_{\text{ox}}$  enhances the contribution of electric field passing through the low dielectric constant  $\text{SiO}_2$  region, thereby reducing  $\kappa_{\text{eff}}$ . Note that  $\kappa_{\text{eff}}$  exceeds the dielectric constant of Si for  $T_{\text{ox}} = 2.5$  nm, which can be attributed to strong screening effects by metallic electrodes ( $\kappa = \infty$ ). These results confirm that the G-kernel captures the dependence of exchange interaction on dielectric environment, demonstrating the strong impact of dielectric inhomogeneity on  $J_{\text{ex}}$ . Since the G-kernel directly incorporates the device-dependent dielectric environment through the Poisson equation, it serves as a physically grounded reference for evaluating exchange interaction.

Finally, we discuss the validity and limitations of the  $\kappa_{\text{eff}}$  approximation for  $J_{\text{ex}}$  calculations. As shown in Figs. 3 and 4, the C-kernel with  $\kappa_{\text{eff}}$  reproduces the G-kernel results remarkably well. Similar agreement has also been confirmed for devices with larger gate lengths and different gate oxide materials. Within the voltage range considered in this study,

this behavior can be understood as follows: although the tunnel coupling changes exponentially with the barrier-gate voltage, the electron distribution varies only slightly, resulting in a nearly constant electrostatic environment. This suggests that the C-kernel with  $\kappa_{\text{eff}}$  can serve as an efficient approximation for estimating  $J_{\text{ex}}$ , provided that the electron distribution does not change significantly during gate operation. However, the approximation can break down under high- $V_{\text{BG}}$  condition where  $V_{\text{BG}}$  approaches  $V_{\text{PG}}$ . Figure 5(a) shows  $J_{\text{ex}}$  for  $W = 24$  nm and  $T_{\text{ox}} = 10$  nm under such conditions, demonstrating a deviation of the  $\kappa_{\text{eff}}$  approximation from the G-kernel results. As the interdot potential barrier becomes extremely low, the electron wave functions are no longer well localized within individual dots. Consequently, the spatial distribution of the electrons changes significantly with  $V_{\text{BG}}$ , as shown in Fig. 5(b). The electrostatic environment experienced by the electrons therefore varies during gate operation, leading to the breakdown of the  $\kappa_{\text{eff}}$  approximation. Although the  $\kappa_{\text{eff}}$  approximation has been shown to provide an effective surrogate model for the  $J_{\text{ex}}$  calculation based on the G-kernel, a reliable procedure for estimating  $\kappa_{\text{eff}}$  without calibration against the G-kernel results is not yet available. The development of simplified methods for estimating  $\kappa_{\text{eff}}$  directly from device structures would further enhance the practical usefulness of the approximation.

#### IV. CONCLUSIONS

A Green's-function-based method for computing the spin exchange interaction  $J_{\text{ex}}$  under an inhomogeneous dielectric environment has been developed, in which geometry-dependent two-electron interactions are accurately treated. Unlike conventional approaches based on a homogeneous Coulomb interaction, the present method captures the device-dependent nature of the interaction arising from dielectric inhomogeneity. Simulations of fin-type Si MOS double quantum dots demonstrate that dielectric inhomogeneity significantly affects the exchange interaction, indicating that the dielectric distribution is a key factor in exchange interaction engineering. The present method provides a physically grounded simulation framework for the accurate design of Si spin qubits toward large-scale integration.

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