# Quantum Algorithms for Simulating Quantum Transport via the Time-Dependent Open-System Schrödinger Equation

Satofumi Souma†
Department of Electrical and Electronic Engineering, Kobe University, Kobe 657-8501, Japan
†email: ssouma@harbor.kobe-u.ac.jp

***Abstract*—We propose and demonstrate a quantum circuit-based framework for simulating quantum transport phenomena governed by the time-dependent Schrödinger equation for open quantum systems. While the theoretical formulation is compatible with large-scale classical simulations, its implementation as a quantum algorithm offers a promising path toward quantum-accelerated modeling of nanoscale devices. A key challenge in such simulations lies in incorporating dissipation and particle injection processes arising from coupling to external reservoirs. In this work, we present quantum circuit constructions that explicitly encode these effects using controlled rotations, measurement-induced decoherence, and reset operations. By comparing the results of our quantum simulations with those obtained from classical numerical solutions of the open-system Schrödinger equation, we confirm that the proposed quantum model can reproduce both transient dynamics and steady-state behavior. These results validate the physical fidelity of the approach and highlight the potential of quantum computing in electronic transport simulations.**

## I. Introduction

In recent years, rapid advances in quantum computing technologies have led to active research on applying quantum computers to real-world problems across various fields. Among quantum computing algorithms, the Quantum Fourier Transform (QFT) and its application, the Quantum Phase Estimation (QPE) algorithm, stand out for their distinct characteristics. These algorithms have long been central topics of research, particularly in solving eigenvalue problems and systems of linear equations [1, 2], and continue to evolve. Moreover, their potential applications are being explored in areas such as quantum chemistry, materials design, and financial engineering, with ongoing efforts to optimize them for specific problems. More recently, research on algorithms tailored for Noisy Intermediate- Scale Quantum (NISQ) devices is progressing rapidly. These algorithms, which utilize hybrid quantum-classical methods, are expected to provide feasible solutions to real-world problems even within the current limitations of quantum hardware.

Notably, variational quantum algorithms (VQAs) have been proposed to solve partial differential equations such as the Poisson equation, which plays a central role in electrostatics and quantum transport modeling of semiconductor devices [3–5]. These approaches leverage the expressive power of parameterized quantum circuits and hybrid quantum-classical optimization to approximate solutions to problems that are otherwise computationally demanding on classical hardware.

Building on this trend, Yang and Guo have recently proposed a variational quantum algorithm tailored for solving the quantum transport equation in semiconductor devices [6]. This work demonstrates the feasibility of incorporating quantum transport formalisms, such as those based on the non-equilibrium Green's function (NEGF) framework [7], into the quantum computing paradigm. Such developments are particularly important in the context of nanoscale transistors, where quantum confinement and tunneling effects dominate charge transport.

In this paper, we explore an alternative approach that applies quantum algorithms to quantum transport simulations based on the time-dependent Schrödinger equation for open quantum systems. While this method is already applicable to large-scale systems using classical numerical solvers [8], translating it into a quantum algorithm may offer future advantages. Furthermore, this approach can be seen as an extension of previously studied quantum algorithms for isolated systems, allowing us to leverage existing insights.

Recent studies have proposed quantum algorithms that directly tackle open quantum system dynamics, such as an efficient scheme using only a single environmental qubit to simulate dissipation [9], and a variational approach for general quantum processes including non-unitary evolutions [10]. These works provide valuable foundations, but they have not been directly extended to model quantum transport phenomena in nanoscale devices with structured environments and spatially resolved observables. Extending the quantum algorithms to transport-oriented open systems necessitates addressing two key elements: the effects of coupling to electrodes and the injection of particles from the electrodes. This study will provide a detailed discussion on potential methods to incorporate these effects into quantum algorithms.

## II. Theoretical method

### *A. Quatntum transport theory based on the time-dependent open-space Shrödinger equation*

The time-evolved state vector in the presence of a perturbation $\hat{H}'$ can be expressed using a Dyson-like integral equation

involving the retarded Green's function $\hat{G}^r$ as:

$$|\Psi(t)\rangle = |\psi(t)\rangle + \int_{-\infty}^{\infty} dt_1\, \hat{G}^r(t,t_1)\, \hat{H}'|\psi(t_1)\rangle, \quad (1)$$

where $G(t,t')$ is the time-dependent Green's function. To describe transport in open quantum systems, it is convenient to partition the system into three regions: the left (L) and right (R) electrodes, and the central device region (C). Then, focusing on the central region and assuming the wide-band limit approximation, we can derive the equation of motion for its wavefunction $|\Psi^C(t)\rangle$ as

$$i\hbar\frac{\partial\,|\Psi^C(t)\rangle}{\partial t} = H^{CC}(t)\;|\Psi^C(t)\rangle + \underbrace{H^{CL}(t)\;|\psi^L(t)\rangle}_{\text{injection from left}} + \underbrace{\left[\Sigma^{(L)}+\Sigma^{(R)}\right]\;|\Psi^C(t)\rangle}_{\text{dissipation}}, \quad (2)$$

where $\Sigma^{(L/R)}$ is the self-energy due to the left/right electrode. By emplying the Crank-Nicolson scheme we obtain

$$|\psi(t+\Delta t)\rangle = \left[1+\frac{i\Delta t}{2\hbar}H'_{\rm C}\right]^{-1}\left[1-\frac{i\Delta t}{2\hbar}H'_{\rm C}\right]|\psi(t)\rangle - \frac{i\Delta t}{\hbar}H_{CL}\,|\varphi_L(t)\rangle\,. \quad (3)$$

with $H'_{\rm C} = H_{\rm C} + \Sigma(\varepsilon)$.

In quantum transport simulations of nanoscale semiconductor devices such as nanowire FETs and nanosheet FETs, it is often reasonable to reduce the problem to a one-dimensional problem along the transport (current flow) direction, where the transverse directions are typically treated in momentum space or using a mode-space approach.

In this approach, the Hamiltonian of the central region consisting of $N$ sites within the finite-difference scheme can be written as:

$$H = \sum_{i=1}^{N}\varepsilon_i\;|i\rangle\langle i| - \sum_{i=1}^{N-1} t_{\rm hop}\left(|i\rangle\langle i+1| + |i+1\rangle\langle i|\right), \quad (4)$$

where $\varepsilon_i$ represents the on-site energy at site $i$, and $t_{\rm hop} = \hbar^2/2m^*a^2$ is the hopping amplitude between nearest-neighbor sites ($a$ is the lattice spacing). The ket $|i\rangle$ denotes the localized state at site $i$ in the position (site) basis. The first term in Eq. (4) describes the potential energy of the system. Then the equation (3) can be solved numerically by using conventional (classical) computers in general.

### *B. Hamiltonian in quatntum algorithm for time-dependent open-space Shrödinger equation*

In quantum algorithm, we employ the single-particle approach, which treats the system as a one-particle problem and directly represents the wavefunction over a discretized real-space basis. For example, a tight-binding Hamiltonian Eq. (4) of dimension $N = 2^n$ can be mapped directly onto an $n$-qubit Hilbert space. In this representation, the quantum state $|\psi\rangle \in \mathbb{C}^{2^n}$ is interpreted as the full wavefunction, and the Hamiltonian Eq. (4) is decomposed into a linear combination of tensor products of Pauli operators:

$$H = \sum_{i=1}^{4^n} c_i\,P_i, \quad c_i = \frac{1}{2^n}{\rm Tr}(HP_i). \quad (5)$$

### *C. Quantum circuit model for an open quantum system with dissipation and injection*

Next we consider a quantum computational model for simulating an open quantum system consisting of a system qubit (single qubit for simplicity) and three types of environment qubits. The full register includes the system qubit $q_{\rm sys}$, a chain of dissipative environment qubits $q_{\rm dis}^{(i)}$ $(i = 0,\ldots,N_{\rm dis}-1)$, a decoherence channel qubit $q_{\rm dch}$, and an injection environment qubit $q_{\rm inj}$.

At each time step $t$, the circuit implements the following sequence of operations. First, the system qubit undergoes unitary evolution via a single-qubit rotation around the $x$-axis:

$$U_{\rm sys}(t) = R_x(\delta\phi), \quad \delta\phi = \omega_{\rm hop}\cdot\Delta t,$$

where $\omega_{\rm hop} = t_{\rm hop}/\hbar$ is the effective hopping frequency derived from a discretized tight-binding model. Next, the system qubit interacts with the dissipative environment. It is first coupled to the leading dissipative qubit via a controlled-$R_x$ gate with angle $\theta_{\rm dis}$, and then the dissipation propagates through the chain of environment qubits via nearest-neighbor CRX gates:

$$U_{\rm dis} = {\rm CR}_x(\theta_{\rm dis}),$$

where we employed $\theta_{\rm dis} = \pi/3$ To model decoherence, each dissipative qubit $q_{\rm dis}^{(i)}$ is further coupled to a shared decoherence channel qubit $q_{\rm dch}$ through a controlled-$R_x$ gate with angle $\theta_{\rm dch}$, followed by projective measurement and reset of $q_{\rm dch}$:

$$U_{\rm dch} = {\rm CR}_x(\theta_{\rm dch}),$$

where we employed $\theta_{\rm dch} = 5\pi/6$.

Injection from the environment is realized by two steps. First, the system qubit is partially entangled with the injection qubit using a controlled-$R_x$ gate:

$$U_{\rm inj,1} = {\rm CR}_x(\theta_{\rm inj}),$$

with $\theta_{\rm inj} = \pi/2$. Then, bidirectional entanglement is established between the injection qubit and the dissipative environment qubits via successive CRX gates:

$$U_{\rm inj,2} = \prod_{i=0}^{N_{\rm dis}-1}\left[{\rm CR}_x(\theta_{\rm inj})_{q_{\rm dis}^{(i)}\to q_{\rm inj}}\cdot{\rm CR}_x(\theta_{\rm inj})_{q_{\rm inj}\to q_{\rm dis}^{(i)}}\right],$$

followed by measurement and reset of the injection qubit.

The combined dynamics of the system under unitary evolution, dissipation, decoherence, and injection are simulated over multiple time steps, with measurement performed at each step to extract the probabilities of the system qubit being in $|0\rangle$ and $|1\rangle$, as well as the occupation states of the environment qubits.

## III. Results and Discussions

Figure 1 presents a reference example to illustrate the basic concepts of potential-induced tunneling and transmission. While this one-dimensional potential barrier is not the main focus of the present study, it serves to highlight the expected quantum mechanical behavior such as wavefunction attenuation and energy-dependent transmission. The corresponding results were obtained using a classical algorithm, and this example is used here solely for illustrative purposes.

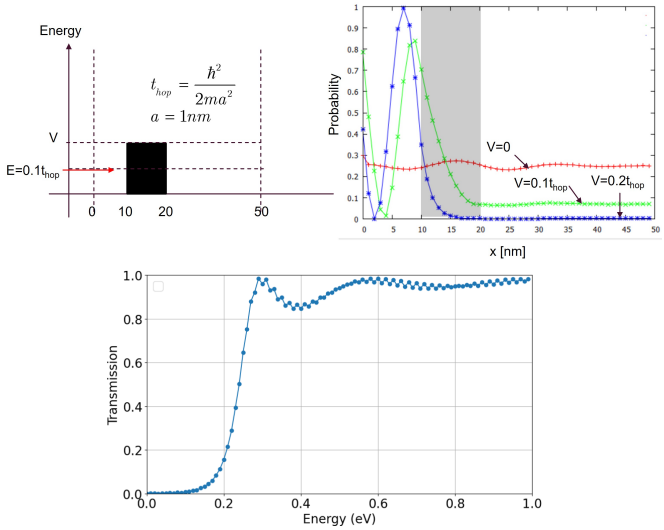


Fig. 1. Fig. 1. (Left) A representative example of the one-dimensional potential barrier considered as a reference case. (Top right) Corresponding probability distributions of the wavefunction for various barrier heights ($V = 0$, $0.1t_{\text{hop}}$, and $0.2t_{\text{hop}}$). (Bottom right) Energy-dependent transmission probability obtained using the classical algorithm. This simple model is shown here for illustration and will not be the focus in the subsequent sections.

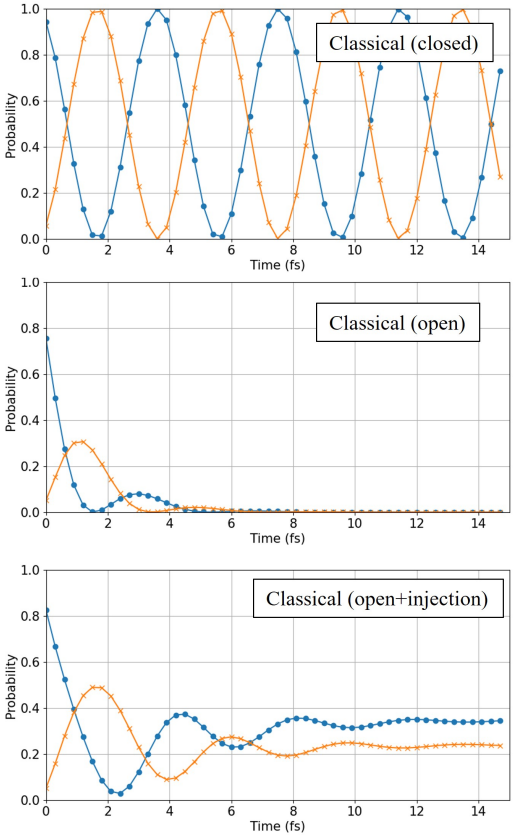


Fig. 2. Time evolution of the probabilities of finding the electron at the left site $|0\rangle$ (blue) and the right site $|1\rangle$ (orange), calculated using the classical algorithm. (Top) Coherent oscillation in a closed two-site system. (Middle) Damped oscillation in an open system with pure dissipation. (Bottom) Non-equilibrium steady-state behavior in an open system including both dissipation and injection from the electrodes.

For the quantum algorithm, since in this study we focus on the conceptual proposal of the quantum algorithm, we restrict first restrict our attention to the two sites $N = 2^n = 2$ ($n = 1$) model with $\varepsilon_i = 0$, $m^* = 0.067m_0$ and $a = 1$ nm.

Figure 2 illustrates the time evolution of the occupation probabilities in a two-level system under three distinct conditions. In the top panel, representing the closed system, the electron exhibits ideal coherent oscillations between the left and right sites, indicating the unitary nature of the time evolution in the absence of environmental coupling. In contrast, the middle panel corresponds to an open system subject to pure dissipation. Here, the amplitude of oscillations decays rapidly, and the probability density vanishes over time, reflecting the irreversible loss of information to the environment and the resulting decoherence.

In the bottom panel, an injection term from external reservoirs is incorporated in addition to the dissipative coupling. As a result, the system evolves toward a non-equilibrium steady state (NESS), characterized by persistent but damped fluctuations around non-zero occupation probabilities. This regime captures the essential features of realistic open quantum transport systems, where decoherence and continuous energy exchange coexist. The distinct behaviors observed across the three panels clearly demonstrate the transition from a fully coherent regime to a decohered, open quantum system with steady-state injection.

Figure 3 presents the results obtained from the quantum circuit model under three different configurations: closed system (top), open system without injection (middle), and open system with injection (bottom). The circuit implementation captures the distinct dynamical behaviors associated with each configuration.

In the closed system case, the expected coherent oscillations are clearly observed, demonstrating coherent population transfer between the two basis states. This behavior is consistent with the classical result, confirming that the unitary part of the system Hamiltonian is faithfully reproduced by the circuit.

In the open system without injection, the quantum simulation exhibits rapid damping of the oscillation amplitude, indicating decoherence due to system-environment coupling. While the transient dynamics show slight fluctuations that are less prominent in the classical simulation, the overall trend-exponential decay toward zero population-is preserved. This confirms that the dissipative effect introduced by the

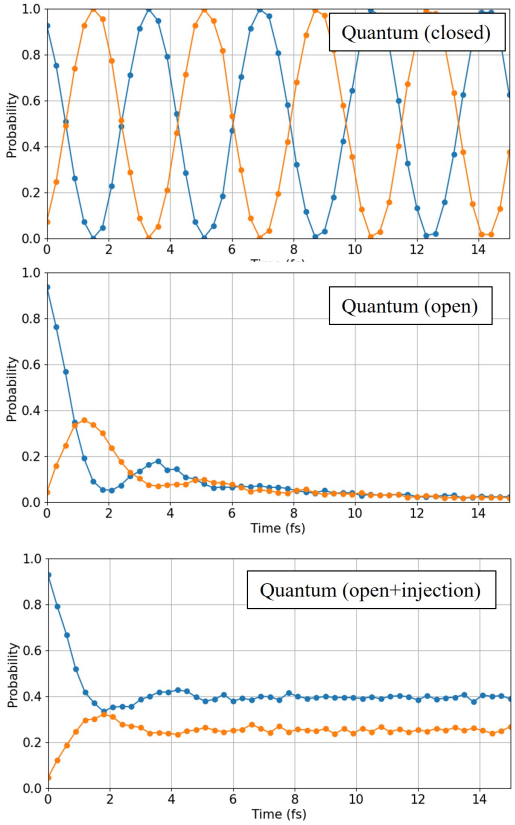


Fig. 3. Time evolution of the probabilities of finding the electron at the left site $|0\rangle$ (blue) and the right site $|1\rangle$ (orange), calculated using the quantum algorithm. (Top) Coherent oscillation in a closed two-site system. (Middle) Damped oscillation in an open system with pure dissipation. (Bottom) Non-equilibrium steady-state behavior in an open system including both dissipation and injection from the electrodes.

measurement-based environment modeling effectively mimics irreversible loss of coherence.

Importantly, in the open system with injection, the quantum model successfully reproduces the emergence of a nonequilibrium steady state. The population probabilities converge to finite values rather than decaying to zero, as expected when continuous inflow compensates for dissipative loss. This steady-state behavior agrees well with that observed in the classical calculation, validating the use of the quantum circuit for simulating transport-like phenomena.

These results collectively indicate that the quantum circuit implementation not only captures coherent dynamics but also effectively models dissipative and driven behaviors in open systems. The long-time behavior, in particular, shows good agreement with classical simulations, demonstrating the capability of the circuit-based approach to approximate the asymptotic regime essential for transport analysis.

## IV. Conclusion

In this work, we proposed a quantum circuit-based framework to simulate quantum transport governed by the open-system Schrödinger equation. By incorporating system-environment interactions via parametrized gates and measurement-based decoherence, we modeled both dissipation and injection processes.

We analyzed system dynamics across three configurations-closed, open without injection, and open with injection-and found good agreement with classical simulations in both transient and steady states. The observed emergence of steady-state behavior highlights the framework's potential to capture nonequilibrium quantum dynamics.

This approach lays the groundwork for simulating transport in nanoscale systems, and future extensions will target multi-site systems and more realistic reservoir dynamics modeling.

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