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Gate-Controlled Electron Quantum Interference Logic Devices

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Abstract

Inspired by using the wave nature of electrons for electron quantum optics, we propose a new type of electron quantum interference logic device (eQILD), where an electron wave is coherently injected into a two-dimensional wave guide and controlled via two gates. Interference effects lead to different current levels in output channels and are utilized for classical logic gates. eQILDs can be reconfigured and support parallelism and multi-valued logic. The operating principle as well as realizations of a logic NAND and NOR gate is shown by means of dynamic quantum Wigner and classical simulations considering coherent/ballistic transport. Contrary to other advanced information processing approaches no magnetic or photonic mechanisms are required. The eQILD is inherently compatible with conventional integrated circuits and thus provides an attractive alternative towards advanced low-power information processing devices with the performance only limited by the single-electron source frequency, i.e., in the GHz regime.

Introduction. By treating electrons as waves, electron quantum optics provides the basis for conducting quantum optics-like investigations in a fermionic picture.^{1,2} Compared to quantum optics, solid-state electron approaches have the advantage in terms of size, scalability, and the ability of the charge degree of freedom to be easily measurable, with the drawback of

a much shorter coherence time. Key enabling technologies are: electron sources (e.g., electron dynamics in a silicon source,³ two-electron sources,⁴ gate-tunable quantum dot in MoS₂⁵), coherent circuits,⁶ and electron detection.⁷ All these technologies are key to electronic quantum applications in sensing,⁸ metrology,⁹ tomography,¹⁰ and information processing (i.e., flying charge qubit systems^{1,11,12}). As is shown in this work, electron quantum optics provides particular exciting opportunities for a novel type of quantum interference devices (QIDs). QIDs have a long history, ranging from superconducting^{13–16} and single-atom¹⁷ approaches to early investigations into logic.¹⁸ In contrast, the here introduced eQILD uses a different operational principle (Figure 1). For the two-dimensional (2D) wave guide we consider a $22 \times 40 \text{ nm}^2$ molybdenum disulfide (MoS₂) single-layer; a 2D semiconductor of the family of transition metal dichalcogenides (TMDCs). The initial choice of MoS₂ is based on excellent transport, fabrication, and insulator compatibility properties and its wide-spread research focus.^{19,20} However, the choice of wave guide material is not limited to MoS₂, other types of 2D semiconductors¹⁹ are in principle compatible with the eQILD design.

The wave guide is insulated by a cap and a substrate layer on the top and bottom, respectively, and offers reflective boundary conditions along $x = 0 \text{ nm}$ and $x = 22 \text{ nm}$ (Figure 2 and 3). The gates are embedded in the cap layer:

Figure 1: Schematic representation of the eQILD. An exemplary potential energy distribution of the wave guide derived from biased gates and the device structure is shown on top. The blue cap layer is partially made transparent to show the inside of the device.

Based on the charge and shape of the gates and the distance between them, the transport domain, the output channel walls (potential energy of 0.1 eV and dimensions $2 \times 10 \text{ nm}^2$ centered at $x = 7 \text{ nm}$ and 15 nm , respectively, and ranging from $y = 30 - 40 \text{ nm}$), and the boundaries, we calculate the corresponding potential energy distribution in the channel as is discussed below (see an exemplary potential energy distribution overlaid in Figure 1). Further considering the physical characteristics of the injected electrons, we use the calculated potential energy distribution to simulate the electron transport (quantum and classical) in the 2D wave guide by stochastic evolution simulations²¹ (see Section Simulation Methodology) for various gate configurations and calculate the current levels in the output channels.

The simulation setup conceptually resembles a double-slit experiment, where single electrons are shot consecutively towards a screen, until a stationary (steady-state) interference pattern is obtained.^{22,23} The probabilistic interpretation is of equivalent independent (uncorrelated) experiments aiming at accumulating sufficient statistics. However, in contrast to the famous double-slit experiments where a single barrier offers two slits, here, similar interference effects manifest by utilizing two potential energy wells in a wave-guide:²² The foundational mechanism of eQILDs. Electrons with energies of 71 meV enter on one side of the device

and cross the device within approximately 200 femtoseconds. The injection frequency of today's single-electron sources can reach 10 GHz,³ which translates to a 100 picoseconds injection period, being orders of magnitudes slower than the electron crossing time: eQILD device performance is thus entirely determined by the performance of the single-electron source.

Single-layer MoS₂ is a direct-bandgap (1.8 eV) semiconductor, which makes it well-suited for low-power applications.²⁴ First principles band structure calculations showed that for n-type single-layer MoS₂ the K, K' valleys, which are well-separated in energy from the satellite valleys, are most relevant for low-field transport. A parabolic band with electron mass $m = 0.48m_0$ (see (1)), with m_0 being the mass of the free electron, gives a perfect description of the conduction band valley around the K point.

The metal gates are each modeled as solid spheres with a radius of 2 nm positioned 3 nm (relative to the sphere center) above the wave guide, resulting in 1 nm cap oxide material (calcium fluoride – CaF₂²⁵) between the surface of the gates and the MoS₂. In the following discussions of the calculated 2D quantum electron densities in the wave guide we consider various gate bias configurations in terms of the electric potential ϕ (potential energy $V = -q\phi$ with q the electron charge): A negative or positive gate bias represents a repulsive barrier or an attractive well for the electrons, respectively.

Simulation Methodology. The numerically solved Wigner transport equation is

$$\left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{r}} \right] f_W(\mathbf{p}, \mathbf{r}, t) = \int d\mathbf{p}' V_W(\mathbf{p} - \mathbf{p}', \mathbf{r}) f_W(\mathbf{p}', \mathbf{r}, t) \quad (1)$$

and corresponds to spatially dependent, electric fields slowly varying in time, so that magnetic effects are not involved.²⁶ Here, t is the time, m the electron mass, $\mathbf{p}$ the momentum, and $\mathbf{r}$ the spatial position; $(\mathbf{p}, \mathbf{r})$ spans the phase space.

Furthermore, V_W is the Wigner potential operator obtained from the electric potential $\phi(\mathbf{r})$ by the Weyl transform and f_W is the Wigner function, providing physical averages by the same expressions inherent for the classical distribution function. The equation fully accounts for coherent, time-dependent quantum effects, such as tunnelling, interference, and non-locality. Despite that (1) can be augmented by terms accounting for decoherence effects of scattering²⁷ here we focus on the coherent behavior, governed by the complicated interplay of the physical characteristics of the electron state in terms of velocity, energy and dispersion, electric potentials and geometry.

We apply the signed-particle model to the Wigner transport equation.²⁸ This model extends the conventional, classical particle model applied in the Boltzmann theory by assigning quantum information to the particles. Quantum particles evolve in a classical way, however, they carry a plus or minus sign, are generated by the Wigner potential V_W , and annihilate each other if they occupy the same point in phase space. Ultimately, we solve the Wigner transport equation by a signed-particle stochastic approach, provided by our ensemble Monte Carlo solver VIENNAWD^{1, 29}

The classical limit of (1) is obtained in the case of slowly varying potentials, when the Wigner potential reduces to the classical force giving rise to the ballistic Boltzmann equation.²⁸ Accordingly, the signed-particle model reduces to the Boltzmann model of classically evolving particles.

An electron is modelled as a minimum uncertainty wave packet, which is described by an admissible Wigner pure state²⁷

$$f_W(\mathbf{r}, \mathbf{p}) = N \exp\left\{-|\mathbf{r} - \mathbf{r}_0|^2 / (2\sigma^2)\right\} \exp\left\{-|\mathbf{p} - \mathbf{p}_0|^2 2\sigma^2 / \hbar^2\right\}, \quad (2)$$

where N is a normalization constant. The state (2) is characterized by a Gaussian distribution³⁰ with a standard spatial deviation $\sigma = 16 \text{ nm}$. This corresponds to a momentum deviation smaller than 0.1 nm^{-1} around

Figure 2: Distribution of quantum electron density [a.u.] for two symmetric gate configurations: $\phi_{G_1} = \phi_{G_2} = 0 \text{ V}$ (a) and $\phi_{G_1} = \phi_{G_2} = 0.21 \text{ V}$ (b). The output channel walls are shown in white. Green circles indicate location of gates.

$p_0 = 0.94 \text{ nm}^{-1}$ and also to an uncertainty of about 5 meV with respect to the kinetic energy of the injected electron.

2D Electron Quantum Transport. Figure 2a considers no applied bias to the gates, Gate 1 (G_1) and Gate 2 (G_2). Electrons are injected in y -direction at the bottom (see green wave-packet in Fig. 1). The two wall potentials impose strong non-local effects upon the electrons, shown in particular by the reduced density in y -direction below the walls. The electron density is thus equally split into the three output channels, following the symmetry of the walls. Figure 2b shows the electron density for a symmetric gate bias configuration, i.e., $\phi_{G_1} = \phi_{G_2} = 0.21 \text{ V}$. The resulting peak of the superimposed electric potential of the two gates, as determined by the gate and device geometry, is 0.17 V on the MoS_2 surface, i.e., both gates act as *attractive* wells. As a result, a focusing effect materializes: The majority of the electron density is guided towards output channel 2 (the central channel).

¹www.iue.tuwien.ac.at/software/viennawd/

Figure 3: Distribution of quantum electron density [a.u.] for two asymmetric gate configurations: $\phi_{G_1} = 0$ V and $\phi_{G_2} = 0.21$ V (a) and $\phi_{G_1} = 0.21$ V and $\phi_{G_2} = -0.21$ V (b). The yellow circle indicates the location of the negatively charged gate.

Figure 3a shows the electron density for an asymmetric gate bias configuration, i.e., $\phi_{G_1} = 0$ V and $\phi_{G_2} = 0.21$ V, corresponding to a resulting peak superimposed electric potential on the MoS₂ surface of 0.14 V, i.e., ϕ_{G_2} acts as an *attractive* well in front of output channel 3 (right channel): The majority of the electron density is thus guided towards channel 3, less so towards channel 2, and considerably less to channel 1 (left channel). Figure 3b shows the electron density for another representative asymmetric gate configuration where the gates are biased in an opposing manner, i.e., $\phi_{G_1} = 0.21$ V and $\phi_{G_2} = -0.21$ V. This configuration corresponds to a resulting peak superimposed electric potential on the MoS₂ surface of 0.11 V in front of channel 1, and a repulsive barrier of -0.11 V in front of channel 3. In this case the electron density guided towards channel 3 is almost completely blocked and the majority of the electron moves towards channel 1; a considerably smaller part of the electron density enters channel 2. We note that the classical picture of the evolution is entirely different, giving rise to different density and current values in the channels, see discussion on quantum versus classical transport below. In particular the effects of penetration and tunneling into the output channel walls seen in both

cases of Figure 3 is a clear indication of the quantum character of the electron evolution.

Gate Control. Figure 4 shows the calculated quantum currents for a representative selection of ϕ_{G_1} biases relative to fixed ϕ_{G_2} biases in the three output channels. The current at the output of each channel has been calculated by integrating the current density along the corresponding output cross-section. In turn, the current density is calculated from the first-order moment of the electron distribution function. Figure 4a considers the case of $\phi_{G_2} = 0$ V; G_2 is thus not active (see a similar scenario in Figure 3a albeit for G_1). For negative ϕ_{G_1} biases, ϕ_{G_1} repulses the majority of the current to channel 3, with a similar inverted behavior for positive biases with respect to channel 1. In case of $\phi_{G_1} = 0$ V, the electron is equally distributed between all three output channels as expected from device symmetry considerations, which corresponds to the scenario depicted in Figure 2a. The negative and positive ϕ_{G_1} bias ranges *seem to offer a mirrored* behavior, however, both ranges correspond to entirely different physical scenarios of repulsion and attraction, leading to different interactions between the electrons and the potential energy landscape and thus to different current levels. Therefore, a fully-mirrored behavior is not to be expected. Figure 4b considers the case of $\phi_{G_2} = 0.105$ V. The negative bias range offers similar general behavior as for $\phi_{G_2} = 0$ V (see Figure 4a), however, for the symmetric case $\phi_{G_1} = \phi_{G_2} = 0.105$ V a focusing effect with respect to channel 2 manifests (similar to Figure 2b). A further increased ϕ_{G_1} bias results in a deeper well potential at G_1 over G_2 , thus the majority of the current manifests in channel 1. Figure 4c considers the case of $\phi_{G_2} = 0.21$ V; G_2 acts as an even stronger attractive well. Yet another intriguing example of quantum non-locality is seen here for negative biases: Although ϕ_{G_2} has doubled (compare with Figure 4b), the current in channel 1 & 2 stays roughly the same but in channel 3 (located behind G_2) is reduced further, demonstrating the wave nature of the evolution.

Figure 4: Output channel quantum currents $I_{C_{1,2,3}}$ for a set of gate biases $\phi_{G_{1,2}}$.

Implementation of NAND/NOR Gates.

Table 1 provides an extended overview of the gate bias to channel current relations and together with Table 2 shows various exemplary interpretations as logic gates: Particularly important are *universal* NAND and NOR gates as both are *functionally complete* and as such can be used to implement all possible Boolean functions.³¹ In classical logic, a NAND gate is defined by the *truth table* $00 \rightarrow 1$, $01 \rightarrow 1$, $10 \rightarrow 1$, $11 \rightarrow 0$ and the NOR gate by $00 \rightarrow 1$, $01 \rightarrow 0$, $10 \rightarrow 0$, $11 \rightarrow 0$, mapping two input states to one output state for the binary-based four configurations. In a similar fashion, additional logic gates can be identified, e.g., AND and NOT gates.

Quantum versus Classical Transport.

Comparative classical simulations (see Section Simulation Methodology) verified that the current is significantly (15-51%) larger in the quantum case. The increased current is due to the wave nature of the electrons, in particular constructive interference. For example, when both gates are driven by 0.105 V, $I_{C_2} = 46 \mu\text{A}$ but the classical current is $28 \mu\text{A}$ ($\sim 39\%$ reduction). An even stronger difference is observed for 0.21 V, where $I_{C_2} = 41 \mu\text{A}$ against a classical current of $20 \mu\text{A}$ ($\sim 51\%$ reduction). A similar behavior is also present for repulsive symmetric potentials: For -0.105 V , $I_{C_2} = 31 \mu\text{A}$ is reduced to $21 \mu\text{A}$ in the classical case ($\sim 32\%$ reduction). Furthermore, in the asymmetric case of $\phi_{G_1} = 0.105 \text{ V}$ and $\phi_{G_2} = -0.105 \text{ V}$, $I_{C_1} = 39 \mu\text{A}$ while the classical current is $33 \mu\text{A}$

($\sim 15\%$ reduction). These significant differences between the quantum and the classical currents clearly show, that indeed quantum effects are essential for eQILDs to allow for more distinct and thus practically usable current levels.

Conclusion. The introduced eQILD provides an alternative path towards advanced non-magnetic, low-power, and high performance classically operating logic devices. The electronic nature of eQILDs provides an attractive alternative path towards co-integration with conventional electronics. The device structure is amenable for fabrication due to simplistic geometries and established materials. Furthermore, various adaptations are perceivable, for instance, additional gates, channels, or bias configurations would allow to introduce even more current states. Alternatively, the output channels can be arranged in a non-symmetric manner or can be merged outside of the device to allow for further superpositioned states. Robustness is tuneable by increasing the current ranges. The eQILD design is in principle adaptable to other transport materials (e.g. other TMDCs), offering additional options for practical realizations. In addition to classical binary logic, the manifestation of several current levels at the individual output channels provides a path towards multi-valued logic, which, although having inherent higher robustness challenges,³¹ promises higher integration densities.³² The fact that different gate bias configurations allow for different current levels allows for reconfiguration:

The same eQILD can realize different logic gates. In addition, only a single output channel is used for realizing a particular logic gate. The fact that additional, specific current levels are available also in the remaining output channels provides a path towards parallelization as various logic operations can be realized in parallel. A particular attractive perspective is provided considering the recent advances towards two-electron sources:⁴ The eQILD operation could be extended towards applications in entangletronics,^{22,33,34} enabling the use of entanglement for non-local classical logic.

Table 1: Output channel quantum currents $I_{C_{1,2,3}}$ (μA) for an extended set of gate biases $\phi_{G_{1,2}}$ (V) relative to Figure 4. The GATE column shows individual rows of the truth tables of realizable NAND and NOR gates according to the rules shown in Table 2; framed current values highlight the utilized channel to realize the logic.

ϕ_{G_1}	ϕ_{G_2}	I_{C_1}	I_{C_2}	I_{C_3}	GATE
-0.21	-0.21	9	10	9	NOR: 11 $\rightarrow$ 0
-0.21	-0.105	10	14	28	
-0.21	0	13	15	36	NOR: 10 $\rightarrow$ 0
-0.21	0.105	16	13	37	
-0.21	0.21	15	14	32	
-0.105	-0.21	28	14	10	
-0.105	-0.105	19	31	19	NAND: 00 $\rightarrow$ 1
-0.105	0	17	11	47	
-0.105	0.105	18	13	39	NAND: 01 $\rightarrow$ 1
-0.105	0.21	16	16	24	
0	-0.21	36	15	13	NOR: 01 $\rightarrow$ 0
0	-0.105	47	11	17	
0	0	26	27	26	NOR: 00 $\rightarrow$ 1
0	0.105	17	13	47	
0	0.21	14	20	34	
0.105	-0.21	37	13	16	
0.105	-0.105	39	13	18	NAND: 10 $\rightarrow$ 1
0.105	0	47	13	17	
0.105	0.105	15	46	15	NAND: 11 $\rightarrow$ 0
0.105	0.21	10	20	40	
0.21	-0.21	32	14	15	
0.21	-0.105	24	16	16	
0.21	0	34	20	14	
0.21	0.105	40	20	10	
0.21	0.21	15	41	15	

Table 2: Exemplary logic gate definitions based on ϕ_G and I_C values of Table 1: IN associates specific $\phi_{G_{1,2}}$ (V) biases with input states **0** and **1**; C is the output channel number; OUT associates specific $I_{C_{1,2,3}}$ thresholds (μA) with output states **0** and **1**; and GATE shows the realizable logic gate.

IN		C	OUT		GATE
0	1		0	1	
0	-0.21	2	≤ 20	> 20	NOR
-0.105	0.105	3	≤ 16	> 16	NAND

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Figures

Figure 1

Schematic representation of the eQILD. An exemplary potential energy distribution of the wave guide derived from biased gates and the device structure is shown on top. The blue cap layer is partially made transparent to show the inside of the device.

Figure 2

Distribution of quantum electron density [a.u.] for two symmetric gate configurations: $\Phi G1 = \Phi G2 = 0V$ (a) and $\Phi G1 = \Phi G2 = 0.21V$ (b). The output channel walls are shown in white. Green circles indicate location of gates.

Figure 3

Distribution of quantum electron density [a.u.] for two asymmetric gate configurations: $\Phi_{G1} = 0V$ and $\Phi_{G2} = 0.21V$ (a) and $\Phi_{G1} = 0.21V$ and $\Phi_{G2} = -0.21V$ (b). The yellow circle indicates the location of the negatively charged gate.

Figure 4

Output channel quantum currents $I_{C1,2,3}$ for a set of gate biases $\Phi_{G1,2}$