



OPEN Implementation of a multi-terminal quantum sorter in solid state systems

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Identifying quantum states stands at the core of quantum information processing. However, an accurate observable measurement can pose a tough challenge whenever multiple outcomes are possible, e.g. measuring momentum vs. electron spin, which takes only two components. Quantum systems with a larger number of degrees of freedom increase the options for quantum computations and may enhance the quantum parallelism. Our goal in this work is to define a system that functions as a quantum sorter in a concrete manner, by choosing an interaction Hamiltonian that enables the device to separate the eigenstates into multiple output ports, achieving a so-called mode-lead disentanglement. To this end, we implemented numerically the R-matrix formalism, which was developed to solve scattering transport problems in solid state systems. The states that are aimed to be separated are described by the transverse momentum of the incident modes and by their spin component, as a possible implementation of qudits. In order to achieve the desired resolution in terms of mode and spin, we study a range of possible Hamiltonians, corresponding to different configurations of the scattering potential.

Information theory stands at the core of technological evolution and has always been a central point of interest in both physics and engineering, the main goal being the realization of devices that perform tasks of information processing more efficiently and at lower physical scales¹. Along with the advent of quantum information in the last decades, the idea that we could harness quantum effects such as interference and entanglement in electronic devices and manipulate qubits for information processing has been a constant objective in physical research^{2,3}.

At the core of quantum information applications, such as logic operations, quantum key distribution and teleportation we invariably have to consider a multi-dimensional Hilbert space to describe the quantum system. For quantum information processing, an essential step relies in the sorting of the multiple degrees of freedom that characterize the system and the subsequent measurements⁴. This has been developed especially in the field of quantum optics, where the study of quantum sorters garnered a large degree of interest, due to their efficiency and applicability in quantum communications and cryptography. These quantum sorters use the photons as the information carriers for different degrees of freedom: polarization and orbital angular momentum^{5–11}, the total angular momentum¹², radial modes^{13–15}, Laguerre-Gaussian modes¹⁶ or spin and radial quantum numbers¹⁷. A number of setups were envisioned, like the full-field mode sorter¹⁸, multimode fiber sorter¹⁹ and all-fiber in-line mode sorter²⁰. All the quantum sorters described above work only for some specific properties of the photons. A generalization of the quantum sorter, which uses any degree of freedom of a D -level system was introduced in Ref.²¹, and it is constructed for a single input port only. Furthermore, a more complex multi-input-port quantum sorter was proposed, which performs the simultaneous sorting of D -level systems^{22,23}.

While photonic qubits pose a series of advantages, such as long coherence times and no requirement for low temperatures during operation, quantum optics based technologies also come with disadvantages, due to the difficulty to manipulate entangled photons and higher optical losses throughout the transmission channel^{24,25}. A central benefit of solid state based quantum computing is scalability and low power consumption, due efficient integration of the quantum computing architectures with the already existing infrastructure of semiconductor-device manufacturing²⁶, taking advantage of quantum mechanical effects like entanglement, tunneling and using spin orbit interaction²⁷. Moreover, in semiconductor structures, charge localization can be controlled with

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relative ease, by means of electrostatic gating²⁸. Solid state physics offers wide a range of promising and versatile implementations for quantum information architectures, from quantum dot qubits to superconducting and topological qubits²⁶. Quantum dots are an exceptional example for the encoding of qubits using charge and spin as degrees of freedom²⁹, especially since the electronic spin in multi-particle QDs has also displayed coherence times that outlive the manipulation time^{30,31}.

In quantum information processing, the qubits are typically employed as elementary information units. Spin-based qubit implementations are most common and the quantum sorters can work as Stern-Gerlach detectors, which have already been proposed³². However, D-level quantum systems, implementing so-called *qudits*, can provide more algorithmic flexibility, enhanced resource-efficiency and parallelism³³. As in the case of qubits, practical realizations of qudits need to account for robustness at decoherence effects, but also for an efficient and reliable detection of the quantum states. Similarly to how photons can be sorted, electrons can also be sorted according to their orbital angular momentum³⁴, which enables more degrees of freedom, i.e. a candidate for a qudit implementation. But, unlike the electron spin, which can accommodate two values, the qudit systems provide a more compact storage of quantum information and open the possibility for processing more complex data structures, potentially reducing the number of computation steps^{35,36}.

In this paper we propose a quantum sorter implementation in a multi-terminal mesoscopic planar device. The incident quantum states are formed by transverse momenta and spin of the electrons in the input waveguide. A tunable scattering potential is used to achieve the optimal conditions for mode-lead pairing in the output leads. One-by-one, the incoming electrons are then scattered preferentially to a certain output lead, depending on the input state. This provides a straightforward method to identify quantum states and their distribution in a more complex signal, by sorting the input states into different output ports and subsequently using particle detectors or simple current measurements in each lead.

Results and discussion

The proposed quantum sorter is a multi-terminal device, built on a high-mobility two-dimensional electron gas (2DEG), which can be realized in quantum wells based on III-V compounds, e.g. using InAs on GaSb substrates³⁷. The QS is operated at low temperatures, typically smaller than 4 K, to preserve the phase coherence length within the device. It has one incoming terminal at the left hand side and four outgoing ones to the right hand side, as it is depicted in Fig. 1. The central scatterer, designed as a triangular shaped region, enables the scattering of the incoming modes into the output leads. Depending on the energy of electrons and on the geometric parameters, corner and side localized states interfere in the scattering region³⁸. A tunable character of the central scatterer is an advantage, as the optimal conditions of mode separation on the outgoing leads is typically hard to anticipate either theoretically or in a practical implementation. In an ideal QS, each incoming mode would be directed towards a separate lead. However, given the complexity of electron scattering in such mesoscopic devices, a more realistic implementation is one of a probabilistic QS, as indicated in Fig. 1a. For a probabilistic QS, there is still a dominant transmission of each incoming mode into a certain output lead, while the remaining leads may also have finite, rather small transmissions. In this case, the mode detection accuracy depends on the ratios between the transmissions in different terminals and, therefore, a certain redundancy in the repeated signal must typically be enforced in order to obtain a correct detection of the incoming state. The schematic representation of the QS, implemented for momentum-spin qudits, is shown in Fig. 1b. Further details about the quantum sorter design are indicated in the Methods section.

In one possible scenario, the particles set on different modes are incoming as separate pulses and one has to determine the type of the mode for each current pulse. In principle, this can be achieved by using only one output lead and observing the different transmission coefficients (currents) for each incoming mode. However, we may be looking at another situation where the four possible signals are mixed: non-interacting particles in all four modes are incoming at very short time intervals apart, possibly overlapping and one has to identify their contributions. Using multiple terminals the four different contributions can be split in the four output leads and thus one may observe in real time the contributions of each incoming mode to the original current (i.e. decompose the mixed signal).

For the implementation of this QS model, there are several key aspects one should consider, which shall be discussed in the following: (i) the ability to discern between incoming states of type $|p_i\sigma\rangle$, (ii) the redundancy in sending a signal and (iii) the stability of the proposed QS configuration with respect to the tunable geometric parameter, h_z , which corresponds to the height of the triangular scatterer.

The accuracy of the QS depends on the distribution of currents in the output ports. Ideally, one incoming mode would be assigned with an output terminal, which would lead to the unambiguous state identification of a single incoming electron. In this case no statistics would be required at the output leads and no redundancy in the signal transmission. However, in typical multi-terminal coherent scattering devices, there is a non-negligible transmission in all output ports. This is due to the fact that the transverse momentum is easily modified in elastic scatterings, making it rather difficult to create a perfect mode-lead pairing in the output leads. Therefore, the relatively broad distribution of significant transmission over the output leads needs to be optimized.

As a criterion, we calculated for the output leads the current ratios between a mode i_1 , and all the other ones, $i_2 \neq i_1$, at given total energy E : $\gamma_I(s, i_1, i_2) = j(s, i_1)/j(s, i_2)$. In our particular system, due to the up-down mirror symmetry enforced by the magnetic barriers on the $|\uparrow\rangle$ and $|\downarrow\rangle$ spins, we determine for $s = 1$ and $s = 2$ two ratios: $\gamma_{I,1} \equiv \gamma_I(1, 0, 1) = j(1, 0)/j(1, 1)$ and $\gamma_{I,2} \equiv \gamma_I(2, 1, 0) = j(2, 1)/j(2, 0)$. Then, we impose that the minimum ratio between the two is above a pre-set threshold, i.e. $\min_s \gamma_{I,s} > \gamma_{\min}$. We consider here an $\gamma_{\min}$ between 5 and 10 to be satisfactory, although higher values are indeed possible. Similarly, one can define the ratio of transmission functions at a given energy, $\gamma_T(s, i_1, i_2) = T(s, i_1)/T(s, i_2)$.

We proceed by tuning the h_z parameter from zero to 200 nm in order to obtain the optimal QS configuration. We find for $h_z = 60$ nm a minimum current ratio $\gamma_{\min} = 10.46$ and we take this case as reference. The

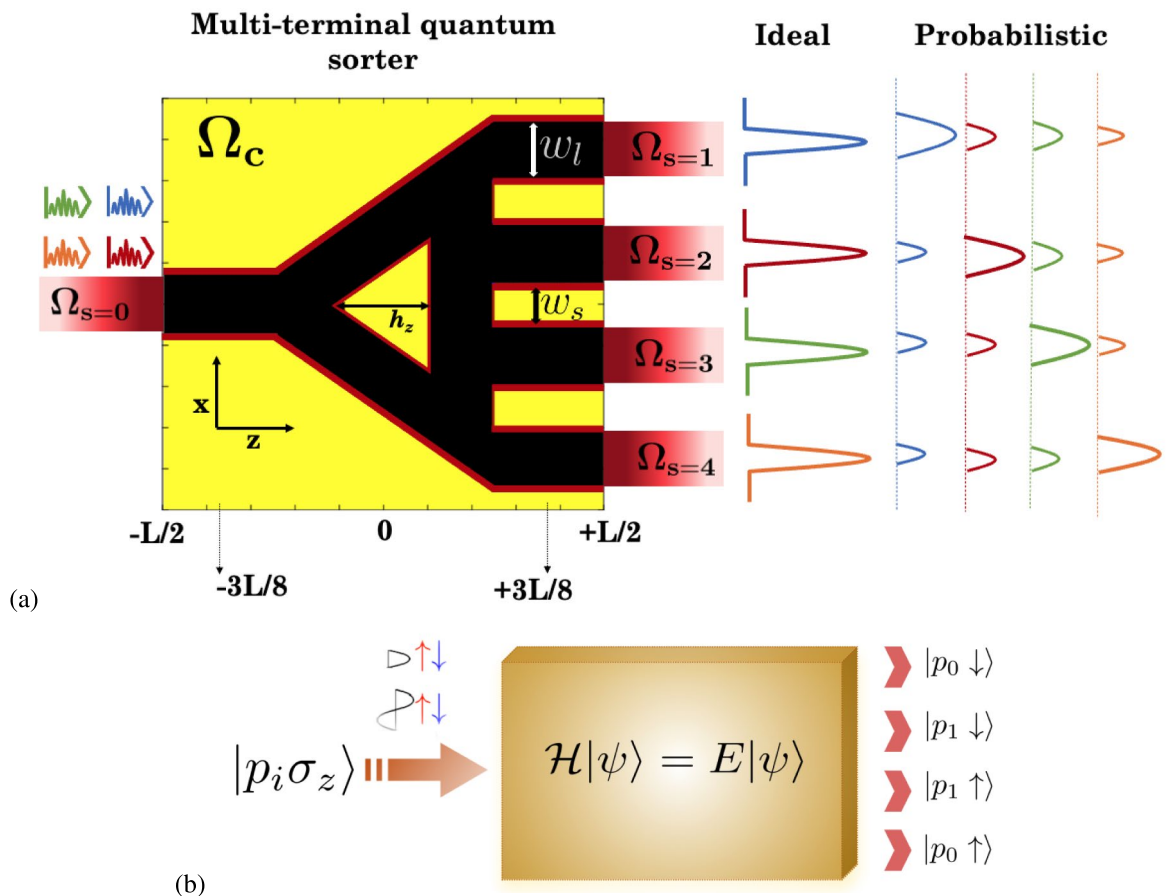


Fig. 1. (a) Multi-terminal design of the quantum sorter (QS): ideal vs. probabilistic QS. There is one incoming lead (Ω_0) on the left hand side and four outgoing leads ($\Omega_{s=1,2,3,4}$) on the right hand side, connected to the scattering region Ω_c ($-3L/8 < z < 3L/8$). Each incoming mode $|p_i \sigma_z\rangle$ is preferentially transmitted on a different outgoing lead. (b) Schematic representation of the QS: two transverse momentum eigenchannels p_i , coupled to spin orientations σ_z , are setting-up the four-state detection experiment.

transmission functions vs. energy for each incoming mode are depicted in Fig. 2. In an energy range of 3 meV to 5 meV we find at $E = 4.04$ meV an optimal device configuration: the mode $|p_0 \uparrow\rangle$ is dominant in $s = 1$, where there is still a small transmission corresponding to second incoming mode, $|p_1 \uparrow\rangle$; in contrast, in lead $s = 2$, mode $|p_0 \uparrow\rangle$ has almost vanishing transmission, while the second mode is well transmitted. Due to the underlying symmetries, this picture is mirrored in the other two leads, $s = 3, 4$. It is worth-noting that, in spite of the complexity of the scattering in the multi-terminal system, the continuous R-matrix model and the tight-binding model implemented by Kwant with a relatively large site-density yield very similar results.

The current and transmission ratios, evaluated on the considered energy range, are shown in Fig. 3. For this reference case, the minimum values for γ_I and γ_T ratios are above 10 and 6, respectively. A more detailed overview on the two ratios around the reference energy is presented in Table 1. We note that for each lead, individually, these values can grow higher and the restriction we imposed, that both transverse modes have the same total energy, lowers the overall detection accuracy. Also, the optimization procedure described here, which relies on a single parameter, namely h_z , is not exhaustive. It merely shows, that by tuning the scattering potential with a single parameter, optimized device configurations can be obtained, which is also a feasible approach in an experimental realization, for instance by controlling a top gate potential.

The second criterion in the QS operation reflects the redundancy in sending the input signal. Even in the case of large current and transmission ratios, γ_I and γ_T , if the transmission coefficients are small, this would correspond to large reflection of the incoming electrons, so that only a fraction of the particles arrive at the left-hand side detectors. In that case, a large number of repetition of the input signal would be required to be able to detect the particles with reasonable confidence rate. In our QS device, from Fig. 2, we see that the transmissions of the two modes are $T_{1,\uparrow} = T_{1,\downarrow} = 0.87$ and $T_{1,\uparrow} = T_{1,\downarrow} = 0.68$, which demands a rather small redundancy. Obtaining very high transmission coefficients in all output leads, for the different input modes, remains one open challenge. By contrast, tunneling systems, with small transmission function, would require high redundancy.

The scattering functions (absolute value squared) for all four incoming modes are visualized in Fig. 4. The rather complex scattering of the transversal modes is captured in the central region. To have a full overview of the scattering process, finite segments of the leads are also depicted, for $|z| > 500$ nm. For each incoming mode,

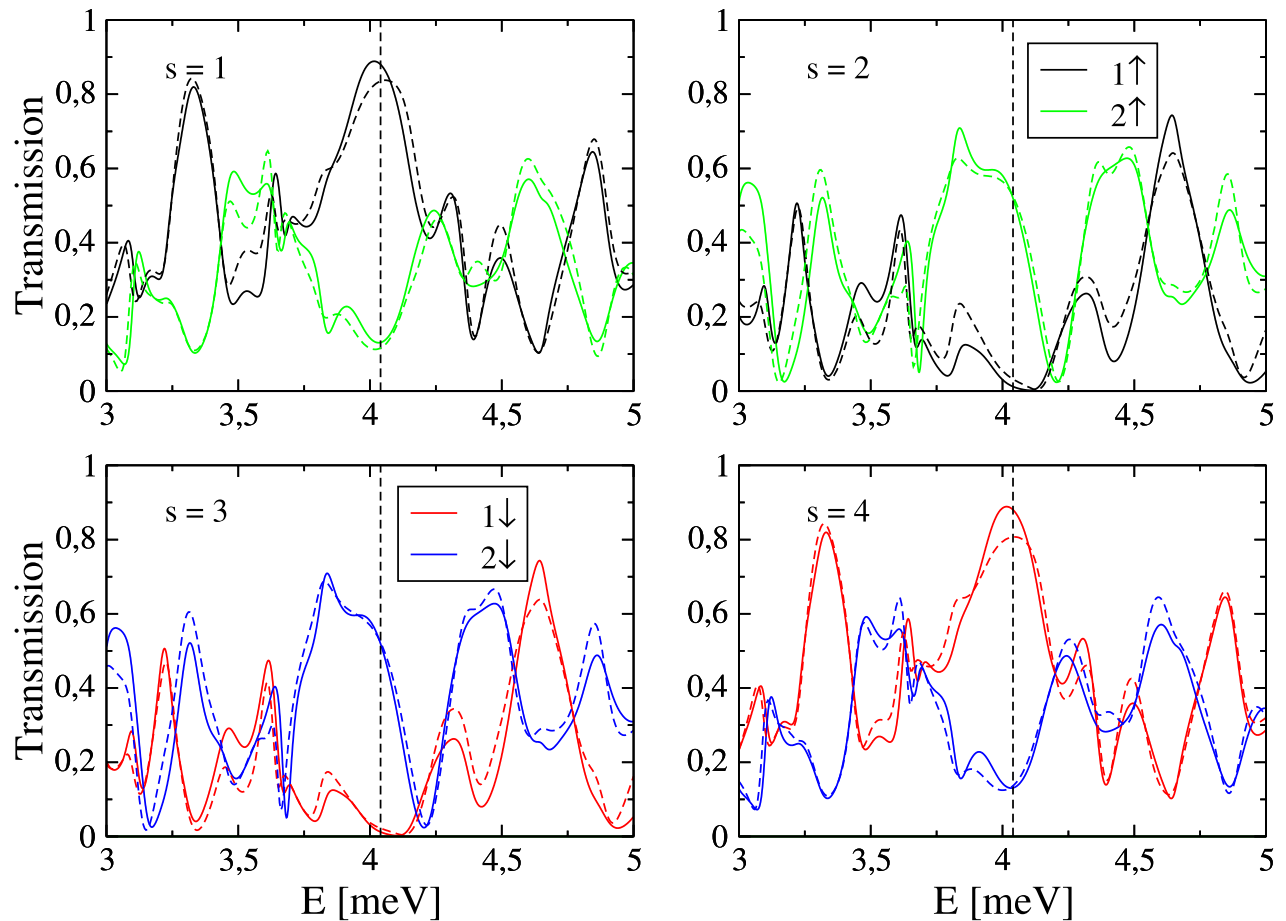


Fig. 2. Transmission functions for each incoming mode, $|p_0 \uparrow\rangle$ (black), $|p_0 \downarrow\rangle$ (red), $|p_1 \uparrow\rangle$ (green), $|p_1 \downarrow\rangle$ (blue), into the output leads, $s = 1, 2, 3, 4$, calculated using the R-matrix method (solid lines). The Kwant calculations (dashed lines) are shown for comparison. The up/down spin symmetry is visible for both transverse modes.

one of the output leads presents a distinctively high transmission in accordance with Fig. 2. Also, the effect of the magnetic barriers is noticeable, as one of the spin components is completely reflected in either upper or lower leads. Again, the underlying symmetries of the system are evidenced. In the output leads, there is a superposition of outgoing modes, i.e. the incident modes are scattered in a combination of available modes.

The third criterion for a practical implementation reflects the stability of a proposed solution. This means that small variations of the tunable parameter around the optimal value would not compromise the QS functionality. To analyze this aspect, we plotted γ_I in Fig. 5a,b for a number of 100 device configurations, as h_z is increased from 0 to 200 nm. In typical resonant systems, sharp features in the transmission function can translate into strong variations of γ_I when the tunable parameter is modified. However, the proposed QS design ensures a minimum γ_I of about ~ 5 , with rather smooth, predictable variations. In particular, around the reference system ($h_z = 60$ nm) we can identify an interval $\Delta h_z \simeq 25$ nm with comparable values of γ_I .

Another, more technical aspect, concerns the convergence of the calculations, which is not easy to achieve in rather complex multi-terminal scattering problems. In the R-matrix calculations, the basis size $N_{bx} \times N_{bz}$ is decisive in performing an accurate calculation, along with the real space grid, $N_x \times N_z$. Therefore, we present two sets of calculations, where, by changing the basis size from 50 to 80 elements on both x and z directions, and increasing the number of grid points from 200×200 to 240×240 , we observe very small variations. Analyzing the γ_I values in Fig. 5a and b we find an overall deviation of only $\sim 13\%$, as mean absolute percentage error (MAPE), when increasing the basis set from 50×50 to 80×80 . Considering also the good overlap of the transmission functions obtained by R-matrix method and Kwant we may conclude that the results are well converged.

We have also checked the variations of current ratios for small deviations of the compensating potential in the magnetic barrier regions, ΔV_Z , from the ideal value and the results are plotted in Fig. 5c. Negative values of ΔV_Z correspond to an effective downshift of energy values (effective quantum wells), while positive values correspond to an up-shift (effective barriers). Over the same energy range, $(-2, +2)$ meV, the relatively small quantum wells affect less the transmission functions compared to the barrier cases, rendering the γ_I ratios almost unchanged. Therefore, in a practical realization of the QS, smaller compensating potentials may be preferred. However, these effects can be further adjusted by the overall tuning of the scattering potential.

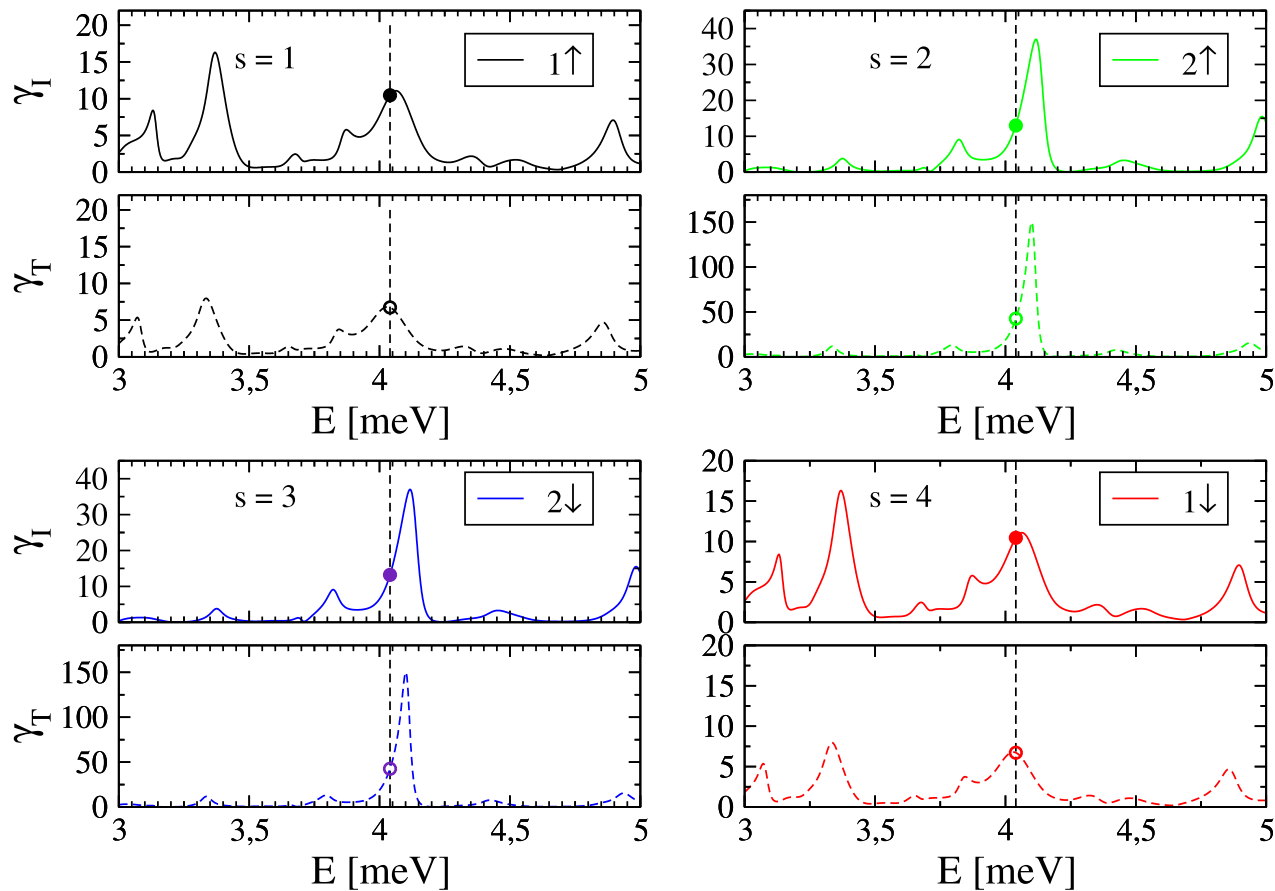


Fig. 3. Ratios of the currents (γ_I) and transmission functions (γ_T), showing the dominant mode transmission in each lead, for an energy of 4.04 meV. Marked with circles are the current ratios $\gamma_I = 10.46$ ($s = 1$), 13.21 ($s = 2$) and transmission ratios $\gamma_T = 6.72$ ($s = 1$), 42.6 ($s = 2$). From symmetry reasons, the other two leads have correspondingly equal values.

Energy [meV]	3.95	4.0	4.04	4.1	4.15	Energy [meV]	3.95	4.0	4.04	4.1	4.15
γ_I 1 $\uparrow$, 1 $\downarrow$	5.15	7.67	10.46	9.43	4.9	γ_T 1 $\uparrow$, 1 $\downarrow$	4.04	6.17	6.72	4.18	1.92
γ_I 2 $\uparrow$, 2 $\downarrow$	3.77	6.5	13.21	33.29	16.35	γ_T 2 $\uparrow$, 2 $\downarrow$	7.92	18.75	42.60	150.1	6.18

Table 1. Current and transmission ratios, γ_I and γ_T , for different modes. From symmetry reasons, equal values are obtained for up and down modes with the same transversal momentum. Overall, high ratios are obtained around the reference energy value or 4.04 eV.

The Kwant calculations confirm the scattering functions maps in fine details, as it is shown in Fig. 6a. Here, only the central regions are depicted. In the tight binding approach, the local current flowing between neighboring sites is illustrated in Fig. 6b. In both figures, the separation of each mode/spin scattering state into one particular output terminal is evident, determined for the energy $E = 3.9$ meV. In spite of the complex scattering problem, the tight binding results are in good agreement with the predictions of the R-matrix simulations in Fig. 4.

The specific design of the QS device, in particular of the central scatterer can be further optimized. In a practical implementation, the top gate can take different shapes, consistent with resolution of the lithographic process. Using the top gate voltage as an external, tunable parameter, the scattering potential can be adjusted in the 2DEG below, so that the optimal conditions for the QS operation are achieved.

Conclusions

We designed a 2D mesoscopic system that works as probabilistic quantum sorter, by choosing a scattering Hamiltonian which enables the device to separate the eigenstates into multiple output ports. In this way, the identification of the incoming quantum states is achieved without a direct measurement of the observables like momentum and spin, but rather by performing a simple particle detection at the output ports. In order to calculate the transmission functions through the system, we implemented numerically the R-matrix formalism for multi-

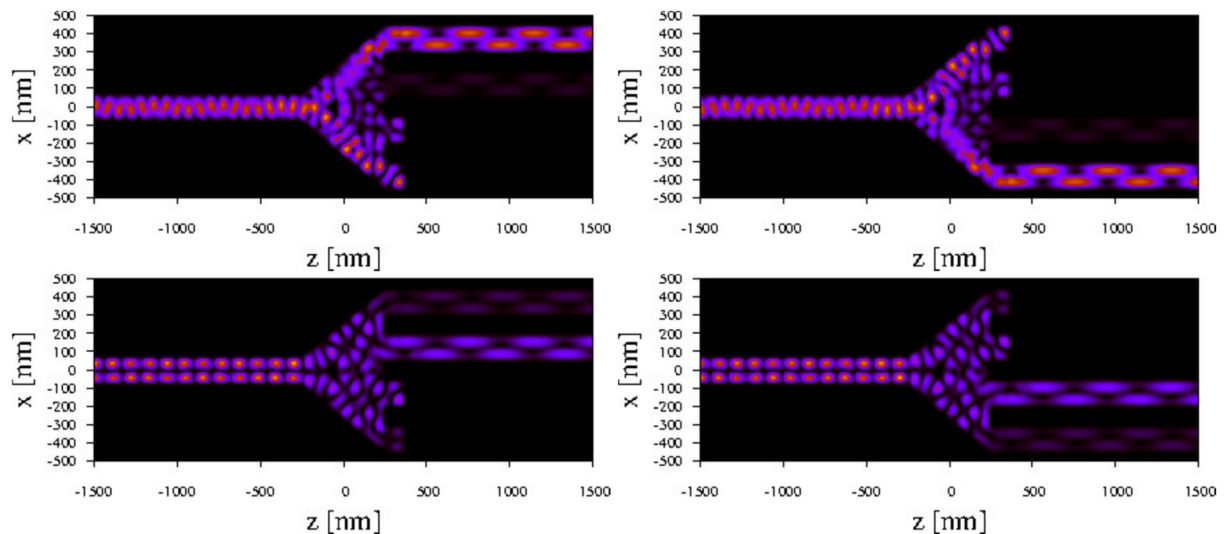


Fig. 4. Wavefunctions (absolute value squared) for the incoming modes, calculated using the R-matrix method. The leads regions are represented for $|z| > 500$ nm. The modes $|p_0 \uparrow\rangle$ and $|p_0 \downarrow\rangle$ (upper row) are mostly transmitted into the outer $s = 1$ and $s = 4$ leads, while the $|p_1 \uparrow\rangle$ and $|p_1 \downarrow\rangle$ (lower row) are scattered to a greater extent into the inner leads ($s = 2, 3$).

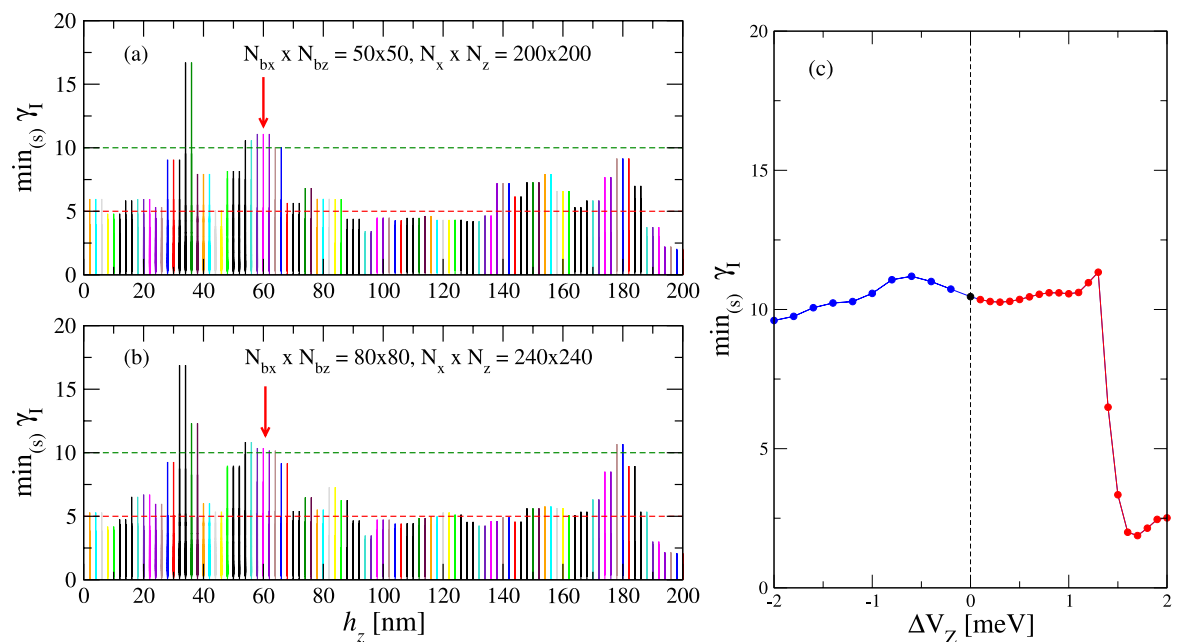


Fig. 5. Robustness of the QS behavior. **a, b** Minimum current ratios for a sequence of $N_{\text{scat}} = 100$ scatterer configurations set by h_z . To check the convergence, two different sets of basis size and grid points were employed: **a** $N_{bx} \times N_{bz} = 50 \times 50$, $N_x \times N_z = 200 \times 200$, **b** $N_{bx} \times N_{bz} = 80 \times 80$, $N_x \times N_z = 240 \times 240$. The red arrows mark the reference system with $h_z = 60$ nm. **c** The stability of current ratios, γ_I , with respect to small changes in the compensating potential, ΔV_z , in the magnetic barrier regions.

terminal transport and compared the results with Kwant calculations in the tight-binding approach. The input states are qudits with four degrees of freedom, defined by their transverse momentum and their spin component. Using a tunable parameter that defines the scattering potential, we optimize the QS device functionality and checked the robustness of the proposed design. This approach can be employed in an experimental realization, where by tuning the gate potential one can determine the optimal operation conditions. Further studies shall be focused on alternative ways to achieve spin separation by electric control, e.g. using Rashba spin-orbit interaction, that would remove the use of magnetic barriers, which are harder to implement experimentally. Moreover, the fragility of the quantum states can be addressed by quantum topological effects which enhance

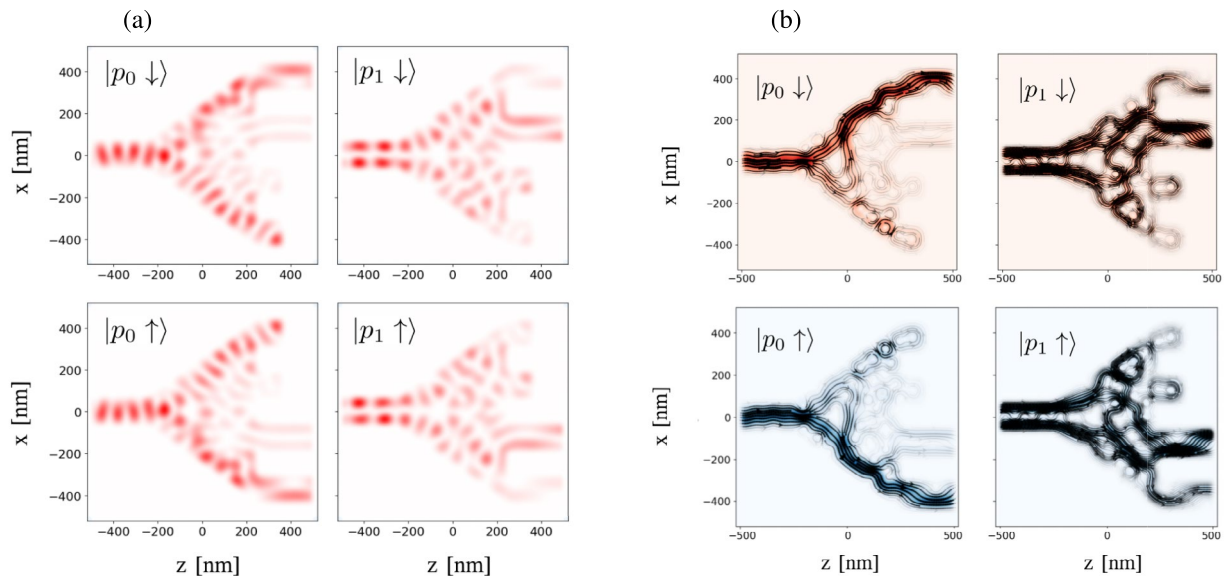


Fig. 6. (a) Wavefunctions (absolute value square) for the incoming modes, calculated using Kwant. (b) Current density maps calculated using Kwant. Both wavefunctions maps as well as the local current distribution, determined using Eq. (19), are consistent with the scattering functions maps shown in Fig. 6. The color gradient corresponds to an increased magnitude of the charge density. The oriented stream-lines indicate the current flow in the QS device..

the resilience to structural disorder and perturbing interactions. Finding a suitable sequence of materials and a proper design is a rather complex task of multi-parameter optimization, which can be further aided by machine learning techniques. Our current investigation is one step for further designing quantum devices that enables proper mode-lead pairing at the output and therefore an efficient quantum state identification.

Methods

Quantum sorter design

As a possible implementation, we considered a square-shaped device in the (x, z) plane of size $L_x = L_z = L = 1 \mu\text{m}$ (Fig. 1a) and divide it into three regions, corresponding to the continuation of the left lead ($z < -3L/8$) and of the right leads ($z > 3L/8$), while in the middle we find the triangular active region of the device. The lead portions of the scattering region have the same characteristics as the semi-infinite leads in terms of potentials and magnetic barriers. The leads are defined by quantum wells with constant potential of width $w_l = 3L/20 = 150 \text{ nm}$, carved out from a base potential barrier of height $V_b = 100 \text{ meV}$. On the receiving end, the three spacers have equal widths $w_s = L/10 = 100 \text{ nm}$. In the active region, the triangular shaped potential barrier drives the electrons sideways, ensuring a more balanced scattering between the inner and outer outgoing leads. The height of this triangle along the incoming lead direction $h_z \leq 200 \text{ nm}$ and it is tuned to optimize the QS operation. In this way we show that, by modifying a single parameter, the QS functionality can be achieved, which is an advantage in practical applications. However, other designs may be envisioned, as the shape of the central scatterer can take different forms, which may be further modified by a top gate voltage. For instance, circular or polygonal scatterers can be produced and customized by electrostatic control of the gates. Furthermore, nanometric fabrication imperfections can be mitigated by fine-tuning of the electronic states using the external voltage control.

In effect, the resulting sharp features in the transmission functions can be exploited to attain a clearer differentiation of the incident modes. For a better separation of the up and down spin components, Zeeman splittings of $V_z = 100 \text{ meV}$ are applied to the right hand side terminals ($z \geq 3L/8$), inducing opposite level shifts for the two pairs of leads positioned above and below the horizontal median ($x = 0$). In addition, to avoid the downshift of energy levels for one spin component, we compensate with an electrostatic potential equal to half of the splitting. In this way, the energy levels corresponding to one of the spin component will remain unchanged, while for the other spin component, the energy levels will shift to higher energies, essentially leading to a cutoff of the respective spin component. In order to enhance the separation of the quantum levels in the rather large confinement area of the device, we considered InAs with a relatively small effective mass, $m^* = 0.023m_0$. InAs quantum wells formed on quasi-lattice-matched (100) GaSb substrates, with high electron mobility of $\sim 2.4 \times 10^6 \text{ cm}^2/\text{Vs}$, constitute a highly performant platform for quantum transport, with reduced parasitic conductance through the substrate³⁷. Furthermore, InAs nanosheets can be transferred on standard Si and GaN substrates³⁹.

The R-matrix method

The coherent transport is described in the framework of the R-matrix method, originally developed by Wigner and Eisenbud⁴⁰, which can efficiently provide the transmission for a wide energy range. Initially, the R-matrix method was used in the study of atomic collisions^{41–43}, while later it became a suitable approach for the investigation of coherent transport of mesoscopic devices^{44–46}. Further on, it was employed to describe the physics of nanotransistors^{46–50}, topological snaking states⁵¹, mesoscopic Aharonov-Bohm effect in gated nanowires⁵², quantum logic gates⁵³ and ballistic neurons⁵⁴ and further developments of the method were performed, concerning time dependent transport⁵⁵, atomistic simulations⁵⁶ and 2-particle scattering⁵⁷.

In the context of the R-matrix formalism, the studied system is divided into two parts - the leads and the scattering (interaction) region. The core idea of the method is that in the scattering region one can write a Schrödinger type of equation, known as the Wigner-Eisenbud problem, and use the eigenfunctions as a basis for the scattering wavefunctions. This part is also the most time consuming because it requires the diagonalization of the system Hamiltonian, with a general scattering potential, which may include Rashba spin orbit interaction, magnetic fields and external electrostatic potentials. In the final step of solving the scattering problem, the R-matrix and scattering matrix are computed, leading to the transmission functions for each of the output leads at given energy.

The time independent Schrödinger equation defines the scattering problem in the entire system:

$$\mathcal{H}\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \quad \mathbf{r} \in \cup_s \Omega_s \quad (1)$$

with asymptotic boundary conditions for the input/output leads.

The Hamiltonian in the scattering (central) region, Ω_c , includes a tunable potential, set by a top gate:

$$\mathcal{H}_c = -\frac{\hbar^2}{2m^*} \Delta + V(\mathbf{r} \in \Omega_c; h_z), \quad (2)$$

which is parameterized by h_z , the height of the triangular shaped scatterer. The interfaces between the scattering region and the leads are planar surfaces denoted by $\Gamma_s = \Omega_c \cap \Omega_s$ ($s = 0, 1, 2, 3, 4$).

The Hamiltonians inside the leads are:

$$\mathcal{H}_s = -\frac{\hbar^2}{2m^*} \Delta + V_s(\mathbf{r} \in \Omega_s), \quad \text{for } s = 0, \quad (3)$$

$$\mathcal{H}_s = -\frac{\hbar^2}{2m^*} \Delta + V_s(\mathbf{r} \in \Omega_s) + V_Z \sigma_z + V_Z \sigma_0, \quad \text{for } s = 1, 2, \quad (4)$$

$$\mathcal{H}_s = -\frac{\hbar^2}{2m^*} \Delta + V_s(\mathbf{r} \in \Omega_s) - V_Z \sigma_z + V_Z \sigma_0, \quad \text{for } s = 3, 4. \quad (5)$$

In Eqs. (3–5) $V_s(\mathbf{r} \in \Omega_s)$ is the confinement potential in the leads, with a longitudinal component that is translationally invariant in the direction of transport and a transverse component which gives rise to the transverse modes in the leads. The term $V_Z \sigma_z$ represents a Zeeman term, which filters the spin in the output leads. The last term, $V_Z \sigma_0$, represents an electrostatic potential that compensates, for one of the spin components, the downshift of the energy levels due to the Zeeman term.

The wavefunctions inside the leads are general solutions of the lead Hamiltonian, namely a superposition between the incident and reflected wavefunctions:

$$\Psi_s(\mathbf{r} \in \Omega_s; E) = \sum_i \Psi_\nu^{\text{in}} e^{-ik_\nu z_s} |\Phi_\nu(\mathbf{r}_\perp, s)\rangle + \sum_i \Psi_\nu^{\text{out}} e^{ik_\nu z_s} |\Phi_\nu(\mathbf{r}_\perp, s)\rangle, \quad (6)$$

where $k_\nu = \frac{\sqrt{2m^*(E - E_\nu^\perp)}}{\hbar}$ are the longitudinal wave vectors and $\nu = (s, i)$ is a composite index with s denoting the lead index, i is the channel index. The functions $\Phi_\nu(\vec{r}_\perp, s)$ are the transverse modes, which are solutions to the following Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m^*} \Delta + V_{\perp, s}(\mathbf{r}_\perp, s)\right) \cdot \Phi_\nu(\mathbf{r}_\perp, s) = E_\nu^\perp \cdot \Phi_\nu(\mathbf{r}_\perp, s), \quad \text{with } |\Phi_\nu(\mathbf{r}_\perp, s)\rangle = \sum_\sigma \Phi_\nu(\mathbf{r}_\perp, s) |\sigma\rangle, \quad (7)$$

where σ is the spin quantum number.

The R-matrix is defined as:

$$R_{\nu\nu'}(E) = -\frac{\hbar^2}{2} \sum_{\sigma, \sigma'} \sum_{l=0}^{\infty} \frac{(\chi_{l, \sigma})_\nu (\chi_{l, \sigma'}^*)_{\nu'}}{E - E_l}, \quad (8)$$

with

$$(\chi_{l, \sigma})_\nu = \int_{\Gamma_s} d\Gamma_s \Phi_\nu(\mathbf{r}_\perp, s) \chi_{l, \sigma}(\mathbf{r} \in \Gamma_s). \quad (9)$$

The functions and energies $|\chi_l\rangle = \sum_{\sigma} \chi_{l,\sigma} |\sigma\rangle$ and E_l are obtained by solving the Wigner-Eisenbud problem:

$$\mathcal{H}_c |\chi_l\rangle = E_l |\chi_l\rangle, \quad (10)$$

with the boundary conditions:

$$\left[\frac{\partial \chi_{l,\sigma}}{\partial z_s} \right]_{\Gamma_s} = 0. \quad (11)$$

The Wigner-Eisenbud functions constitute a basis set for scattering functions inside the scattering region:

$$\Psi(\mathbf{r} \in \Omega_c; E) = \sum_{l,\sigma} a_l(E) \chi_{l,\sigma} |\sigma\rangle. \quad (12)$$

The scattering functions inside the leads, $\Psi_s(\mathbf{r} \in \Omega_s; E)$ and inside the central region, $\Psi(\mathbf{r} \in \Omega_c; E)$, as well as their normal derivatives obey the continuity relations at the $\Gamma_s = \Omega_c \cap \Omega_s$ interfaces, $\Psi|_{\Gamma_s} = \Psi_s|_{\Gamma_s}$ and $\Psi'|_{\Gamma_s} = \Psi'_s|_{\Gamma_s}$, respectively. From this system of equations, the scattering matrix $S(E)$ is identified in terms of the R matrix:

$$S(E) = - \left[1 - \frac{i}{m^*} R(E) k(E) \right] \left[1 + \frac{i}{m^*} R(E) k(E) \right]^{-1}, \quad (13)$$

where k is a diagonal matrix with elements $k_{\nu\nu'} = k_{\nu} \delta_{\nu\nu'}$. Then, the scattering wavefunctions inside the leads and scattering region can be obtained for a given total energy⁵⁵.

The total transmission in lead s for an incoming mode $\nu' \equiv (s' = 0, i')$ is calculated from the symmetric $\tilde{S} = k^{1/2} S k^{-1/2}$ matrix:

$$T(s, i') = \sum_i |\tilde{S}_{\nu\nu'}|^2. \quad (14)$$

The cross-section-averaged current density for the input port ($s' = 0$) is

$$j_0 = j_0^{\text{in}} - j_0^{\text{out}} = \frac{\hbar}{m^*} \sum_{i'} (|\Psi_{0,i'}^{\text{in}}|^2 - |\Psi_{0,i'}^{\text{out}}|^2) k_{0,i'} \quad (15)$$

and, for the output ports ($s = 1, 2, 3, 4$),

$$j_s^{\text{out}} = \frac{\hbar}{m^*} \sum_i |\Psi_{\nu}^{\text{out}}|^2 k_{\nu}. \quad (16)$$

Tight binding simulations

Along with the R-matrix method, we also employed a complementary approach based on the tight binding model. To this end, we used Kwant⁵⁸, an intuitive and versatile Python library that focuses on quantum transport calculations and employs the wavefunction matching method to solve scattering problems. The quantum sorter device was recreated using a square lattice with a single atom basis as a template, setting the lattice constant a at the same dimension of the grid in the R-matrix numerical model. Given the linear size $L = 1 \mu\text{m}$ and the number of grid points $N_x = 200$, the grid size in both descriptions is $a = 5 \text{ nm}$. We ensured that the potential profiles in both simulations are identical, since the resulting transmission of this mesoscopic system is highly sensitive to any variation in the geometrical characteristics. The tight binding version of the system Hamiltonian is the following:

$$\mathcal{H} = \sum_{\langle ij \rangle, \sigma \sigma'} t^{\sigma \sigma'} \sigma_0 |i, \sigma\rangle \langle j, \sigma'| + \sum_{i \in S, \sigma \sigma'} V_i \sigma_0 |i, \sigma\rangle \langle i, \sigma'| + \sum_{i \in Z, \sigma \sigma'} \frac{g \mu_B}{2} \mathbf{B} \cdot \boldsymbol{\sigma} |i, \sigma\rangle \langle i, \sigma'|, \quad (17)$$

where t is the hopping parameter, the sum over $\langle ij \rangle$ indicates that it is taken over nearest neighbors only, $(\sigma_0, \boldsymbol{\sigma})$ stand for the identity matrix and the Pauli vector that incorporates the Pauli matrices, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, and $\mathbf{B}$ is the external magnetic field. S stands for the whole scattering region and Z denotes the area where the Zeeman term is applied (see Fig. 7b). In contrast to the R-matrix simulations, for the Kwant simulation we only applied the in-plane Zeeman field in a narrow region before the boundary with the semi-infinite leads (Fig. 7b).

The mode and spin resolved transmission functions were obtained solely from the unitary S-matrix that is the main output of the tight binding code and we can see that they are highly similar to the transmissions from the R-matrix simulations (Fig. 2). To obtain the spin resolved charge density, we used the following formula, already implemented in Kwant⁵⁸:

$$\rho_{\sigma}^i(E) = \sum_a \begin{pmatrix} \psi_{a\uparrow}^{i\dagger}(E) \\ \psi_{a\downarrow}^{i\dagger}(E) \end{pmatrix}^T \mathbf{P} \begin{pmatrix} \psi_{a\uparrow}^i(E) \\ \psi_{a\downarrow}^i(E) \end{pmatrix} \quad (18)$$

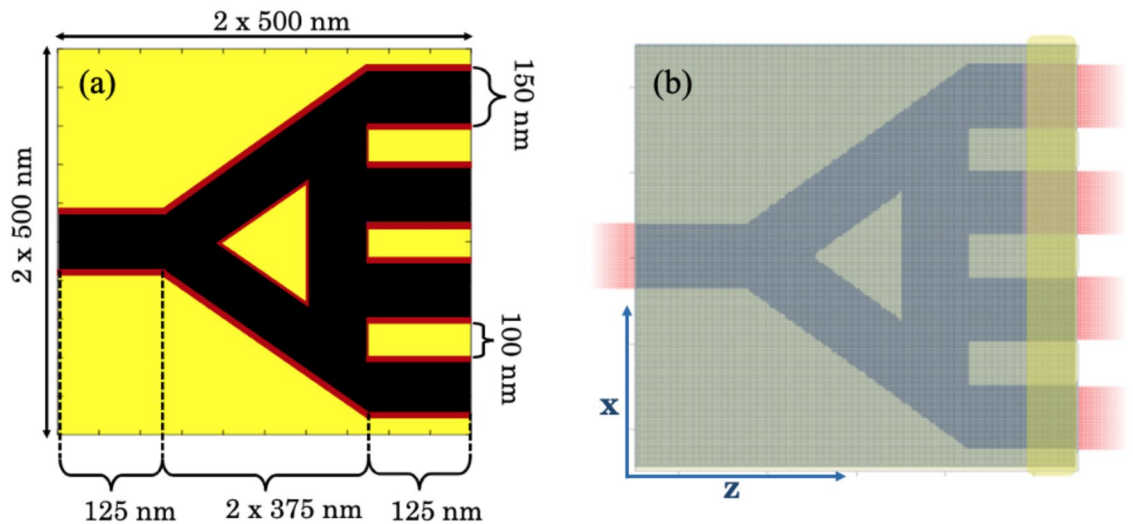


Fig. 7. The potential map in the scattering region, with a triangular scatterer: (a) continuous model in the framework of the R-matrix method and (b) tight-binding model, implemented with Kwant, showing the positioning of magnetic barriers (yellow) and the attached leads (red).

where a stand for the lattice site, E is the energy and i is the mode of the scattering state and $\mathbf{P}$ is an operator corresponding to the observable we are interested in computing (in our case, $\mathbf{P} = \sigma_z$). Employing the same quantities, one can also define local current flowing from site b to site a ⁵⁸:

$$J_{ab} = i \left(\psi_b^\dagger (\mathcal{H}_{ab})^\dagger \mathbf{P} \psi_a - \psi_a^\dagger \mathbf{P} \mathcal{H}_{ab} \psi_b \right), \quad (19)$$

where $\mathcal{H}_{ab}$ is the hopping matrix from site b to site a .

The current tensor displayed in Eq. (19) is a discrete representation of the current density field, where the current density is non-zero only along the lines that connect neighboring lattice sites coupled through the hopping Hamiltonian. In current density plots, the arrow direction indicates the direction of the current flow (oriented stream-line), given by the gradient of the scattering wavefunctions. For appropriate visualization of the scalar current field, the Kwant plotting libraries⁵⁸ have integrated a smoothing term that results in an interpolated current, which is represented for our system in Fig. 6b.

Data availability

All data generated or analyzed during this study are included in this published article.

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Author contributions

A.T.P., I.G., and G.A.N. contributed to the conceptualization and the methodology. A.T.P. and G.A.N. contributed to the investigation. A.T.P. and G.A.N. contributed to writing the original draft. L.I., U.W. and A.M. contributed to writing the review and editing. All authors have given approval to the final version of the manuscript.

Declarations

Competing interests

The authors declare no competing interests.

Additional information

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