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Study on Physical Characteristics and Quantum Transport Law in Low-dimensional Quantum System

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Abstract

As electronic devices continue to shrink to nanometer scale, low-dimensional quantum systems have become the core platform for condensed matter physics and the development of next-generation technology. In this paper, the physical properties and quantum transport laws of low-dimensional quantum systems are systematically reviewed. Firstly, the low-dimensional structures are classified according to the effective dimension (0D/1D/2D), and their characteristic electronic structures, density differences of states and key physical phenomena are summarized. Next, the main theoretical tools of quantum transport are introduced, including the Landauer–Büttiker formula and the non-equilibrium Green's function method, along with discussions on representative mechanisms such as ballistic transport, quantum tunneling, Coulomb blockade, Kondo effect, and topological edge state transport. Further analyze the dimension-dependent transport characteristics, external field regulation behavior, topology and spin-related transport, and the latest progress of molecular-scale quantum interference effect. This paper aims to provide concise reference for researchers entering this field and stimulate interdisciplinary exploration.

Keywords

Low-dimensional quantum system; Quantum transport; Quantum confinement effect; Topological edge state; Coulomb blockage.

1. INTRODUCTION

Electronic devices continue to shrink to the nanometer scale, which has profoundly changed the research pattern of condensed matter physics, making low-dimensional quantum systems the core platform for exploring basic physics and developing the next generation technology. When the spatial scale of the material is reduced to the length of the carrier de Broglie wave, the quantum confinement effect dominates, resulting in discrete energy levels, changing the abnormal density, and exhibiting novel electrical, optical and magnetic properties that do not exist in bulk materials [1]. In the past decades, low-dimensional nanostructures such as 0D quantum dots, 1D nanowires/carbon nanotubes, 2D quantum wells/graphene/transition metal chalcogenides have been widely studied, revealing a large number of emerging phenomena.

Among the rich physical properties of low-dimensional systems, quantum transport behavior is a key bridge connecting micro-quantum mechanics with macro-device functions [2]. At mesoscopic and nanoscale, the charge transport can no longer be fully described by classical Ohm's law. Quantum coherence, electron correlation, spin-orbit coupling and topological protection jointly determine the conductance, noise and thermoelectric response of the system [3]. Milestones such as the whole/fractional quantum Hall effect in 2D electron gas, the quantization of conductance in quantum dot contact, Coulomb blocking in single electron

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transistor and ballistic transport in carbon nanotubes have not only deepened the understanding of quantum mechanics, but also paved the way for practical applications such as quantum computing, low-power electrons and energy collection.

In this paper, the physical properties and quantum transport laws of low-dimensional quantum systems are systematically reviewed. Firstly, the low-dimensional structures are classified according to the effective dimension (0D/1D/2D), and their characteristic electronic structures and key physical phenomena are summarized. Then the main theoretical tools of quantum transport are introduced, and the representative mechanisms such as ballistic transport, quantum tunneling, Coulomb blocking, Kondo effect and topological edge state transport are discussed, emphasizing their dimensional dependence. Further highlight the latest progress in field effect control, spin-dependent transport and quantum interference effect in molecular junction/van der Waals heterojunction. It is hoped that this paper will provide concise reference for researchers entering this field and stimulate more interdisciplinary exploration.

2. CLASSIFICATION AND BASIC PHYSICAL CHARACTERISTICS OF LOW-DIMENSIONAL QUANTUM SYSTEMS

Low-dimensional quantum systems are mainly divided into 0D, 1D and 2D according to the spatial dimension of electron confinement. The difference of confinement dimensions directly leads to the significant difference of electron density of state [4], which further determines the unique electrical, optical and thermal properties of materials. Table 1 below compares the core physical parameters of the three systems and briefly summarizes their basic physical characteristics.

Table 1. Comparison of core physical parameters of different dimensional systems

Dimension	Typical representative	Density of states characteristics	Bandgap characteristics	Typical dimensions/structural features
0D	Quantum dots, nanoparticles	Atomically shaped	Discretization, size determines gap size	Space is limited in three dimensions, typically ranging from 2-10 nm in size
1D	Nanowires, carbon nanotubes	van hove singularity	Quasi continuous, with bandgap present	Two dimensional constraint, with length far greater than diameter
2D	Graphene, quantum well	Stepped	Affected by quantum confinement effect, bandgap can be controlled	Only 1D restricted, with a thickness of about atomic level (<1 nm)

0D system is quantum confined in three directions in space, and the electronic energy level is completely discrete, showing the characteristics of "artificial atom". Its most striking feature is that the density of states is sharp δ-function (as shown in Figure 1), which leads to a high concentration of electron transition energy. This makes quantum dots exhibit strong size-dependent optical characteristics and nonlinear optical response, and Coulomb blocking effect is particularly significant because of the separation of energy levels, which is the core physical basis of single electron transistors.

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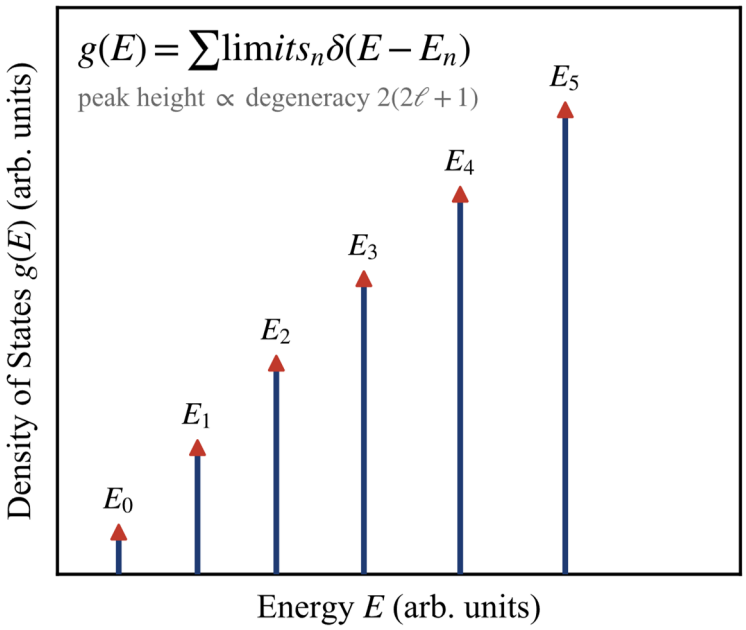

Figure 1. Function-like state density of 0D quantum dots

1D system is confined only in the radial direction, and electrons are confined to a single channel along the axial direction. Its electronic structure is strongly anisotropic, and the density of states presents divergent Van Hof singularity at a specific energy. Limited by 1D channel, electron scattering is greatly suppressed, and ballistic transport is easy to realize, showing extremely high conductivity. At the same time, the limited geometric structure is easy to induce lattice distortion, produce Peierls phase transition, and significantly enhance electron-phonon coupling [5], so that 1D systems often show unique superconducting or charge density wave characteristics.

The 2D system is confined only in the vertical direction, and electrons move freely in the plane, forming a quantum well structure. The density of states presents a step distribution, and each step corresponds to the opening of a subband. This kind of material not only has very high carrier mobility, but also the quantum interference effect and quantum Hall effect are particularly significant due to the decrease of dimensions. In particular, the Dirac material [6], represented by graphene, exhibits massless Dirac fermion characteristics under low-energy excitation, ultra-high electron mobility and unique chiral transport properties. In addition, the bonding between layers of 2D layered materials by van der Waals force provides an excellent platform for building artificial heterojunction by stacking, which greatly expands the regulation space of energy band engineering.

3. THEORETICAL FRAMEWORK AND METHOD OF QUANTUM TRANSPORT

3.1. Basic theory of quantum transport

The transport of electrons in low-dimensional system needs to be described by quantum mechanics, and its core lies in treating the device as an open system model of "central region-electrode". When the average free path of electrons is larger than the device size, the transport is in the ballistic transport region, at which time the scattering can be ignored and the electrons propagate coherently in the form of waves.

The most classical theoretical framework for describing ballistic transport is Landauer-Büttiker formula [7]. This formula directly relates the conductance to the electron transmission

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probability. Under the linear response of zero temperature and small bias, the conductance of the two-port system can be written as:

$$G = \frac{2e^2}{h} T(E_F) \tag{1}$$

Where $T(E_F)$ is the transmission coefficient at Fermi level. For multi-port system, Boutique extended it to:

$$I_i = \frac{2e}{h} \sum_j \int dE T_{ij}(E)\left[f_i(E) - f_j(E)\right] \tag{2}$$

The formula successfully explains the experimental phenomena such as conductance quantization in quantum dot contact.

When the system involves electron-electron interactions, inelastic scattering, or is far from equilibrium, the Landauer formula is no longer applicable, and the non-equilibrium Green's function (NEGF) method must be used. Based on Keldysh contour technique, NEGF describes the propagation and occupation of electrons in an open system by delaying Green's function G^r, leading Green's function G^a and Keldysh component $G^<$. The current is given by Meir-Wingreen formula:

$$I = \frac{2e}{h} \int dE \mathrm{Tr}\left[G^r(E)\Gamma_L(E)G^a(E)\Gamma_R(E)\right]\left[f_L(E) - f_R(E)\right] \tag{3}$$

Where $\Gamma_{L,R}$ is the line width function of the left and right electrodes, which indicates the coupling strength between the electrodes and the central region. NEGF framework can deal with elastic and inelastic scattering, finite temperature and multi-body interaction in a unified way, and it is the mainstream method for quantum transport simulation of nano-devices.

3.2. Key physical effects

A variety of unique transport effects have emerged in low-dimensional quantum systems, and several representative mechanisms are listed below:

(1) Quantum tunneling effect

When the electron energy is lower than the barrier height, due to wave-particle duality, electrons still have a certain probability to penetrate the barrier and form tunneling current. The tunneling probability is obtained by Wentzel–Kramers–Brillouin (WKB) approximating or accurately solving the Schrodinger equation [8]. In the double barrier structure, electrons can form a quasi-bound state in the potential well. When the incident electron energy resonates with the quasi-bound state, the transmission probability increases sharply, and resonance tunneling occurs, and the current presents an obvious peak structure (Figure 2).

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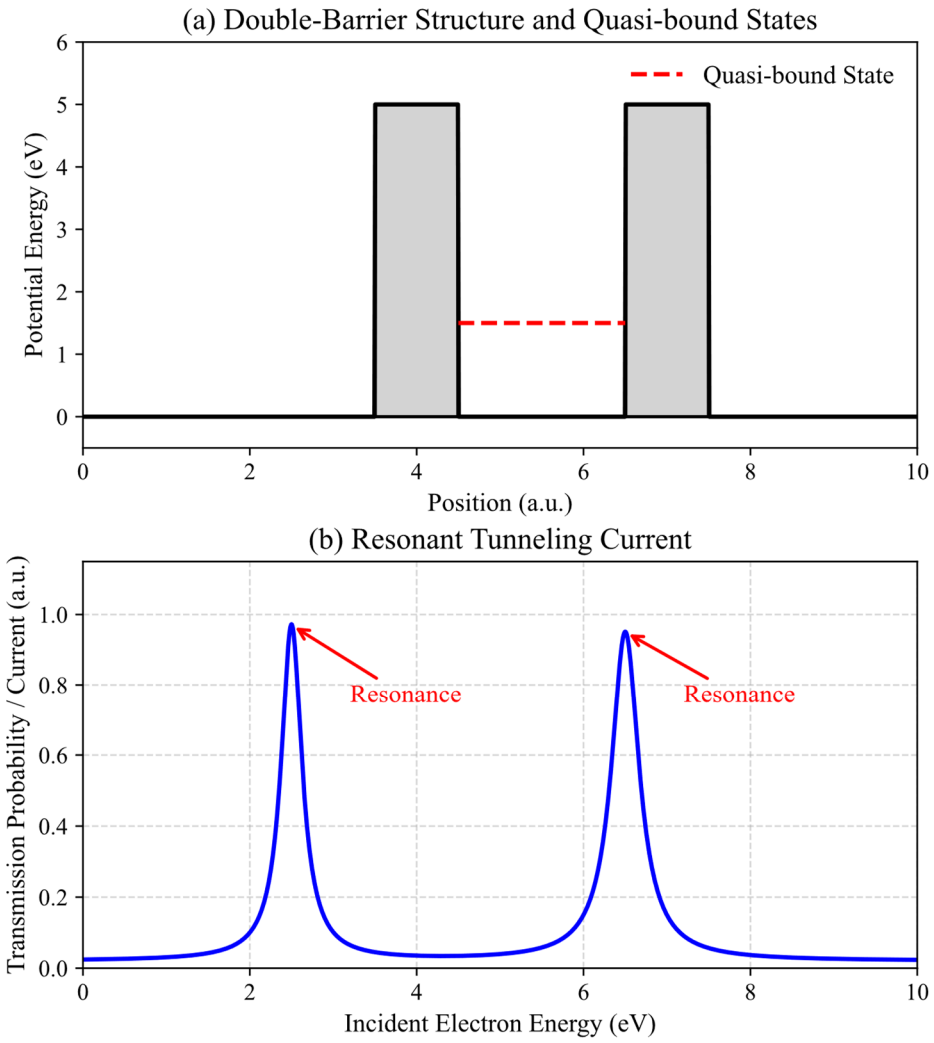

Figure 2. Resonance tunneling phenomenon of double barrier structure in quantum tunneling effect

(2) Coulomb blocking effect

In 0D structures such as quantum dots, the charging energy $E_C = e^2/2C$ of a single electron may be much greater than the thermal energy $k_B T$. At this time, the electron tunneling into the quantum dot will significantly change its electrostatic potential, form an energy barrier, prevent the subsequent electron tunneling, and cause the current to be "blocked". When the gate voltage is adjusted to align the quantum dot electrochemical potential with the electrode, the blocking is lifted, and the current peaks, forming Coulomb oscillation. This effect is the physical basis of nano-devices such as single electron transistor (SET).

(3)Kondo effect

When there are unpaired local spins in quantum dots, conduction band electrons and local spins are antiferromagnetically coupled, forming a narrow Kondo resonance peak near Fermi level, which significantly enhances the low-temperature conductance [9]. Kondo temperature T_K represents the characteristic energy scale of this effect and satisfies $T_K \propto \exp\left[-\pi U/\left(\Gamma_L + \Gamma_R\right)\right]$, where U is Coulomb repulsion energy. Kondo effect embodies the rich physics of associated electron transport in low-dimensional system.

(4) Topological edge state transport

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In 2D systems such as topological insulators, there is an energy gap in the posture, but there is a conductive edge state at the boundary protected by topology [10]. These edge states have spin-momentum locking characteristics, backscattering is suppressed, transport presents perfect ballistic behavior, and they are immune to nonmagnetic impurities. This mechanism provides a new way for quantum transport with low dissipation and spin polarization.

3.3. Common numerical/analytical tools

The theoretical calculation of quantum transport depends on a variety of numerical and analytical methods, each of which has its own scope of application (see Table 2).

Table 2. Theoretical calculation method of quantum transport

Method	Core idea	Applicable scenarios
Tight binding model+NEGF	Discretize the system into lattice points, construct a Hamiltonian, and solve the Green's function using the Dyson equation	Mesoscale nanowires, graphene nanoribbons, molecular structures, etc
Scattering Matrix (S-matrix) Method	Transform the transport problem into solving the scattering state under open boundary conditions, and obtain the transmission coefficient by matching the wave function	Ballistic transport, 1D/2D waveguide
Recursive Green's Function (RGF) algorithm	Using the block tridiagonal structure of Hamiltonian to recursively calculate Green's function, significantly reducing computational complexity	NEGF calculation of large-scale 2D systems
KWANT software package	Open source tool based on Python, using tight binding model and scattering matrix method, can efficiently calculate conductivity, density of states, etc	Rapid prototyping design, instructional demonstrations, complex geometric structures
First principles+NEGF (DFT+NEGF)	Calculate electronic structure using density functional theory, combined with NEGF for transport processing	Atomic level precision simulation of real material devices
Quantum Master Equation (QME)	Establish the equation of motion for the density matrix of open quantum systems and handle time-dependent and non-equilibrium transport under weak coupling	Time dependent dynamics and strong correlation effects in quantum dots and molecular structures

In practical research, the choice of method depends on the system size, interaction strength and required accuracy. For large-scale systems with weak interaction and phase coherence, tightly bound NEGF or scattering matrix method is more efficient; For real materials that need atomic precision, DFT+NEGF is the first choice; For strongly correlated systems, more advanced methods such as quantum master equation or numerical renormalization group (NRG) are needed.

4. RESEARCH PROGRESS AND DISCUSSION ON QUANTUM TRANSPORT LAW

4.1. Dimension-dependent transport characteristics

The transport properties of low-dimensional systems are determined by the density of states (DOS) and the dimensional dependence of scattering mechanism [11]. In 0D quantum dots, the

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energy levels are completely discrete, and the transport shows single electron tunneling and Coulomb blocking steps. The 1D system has Van Hoff singularity, which is prone to Luttinger liquid behavior, and the conductance presents a quantized platform, and the backscattering is suppressed. 2D materials exhibit a unique linear or parabolic dispersion relationship, and its weak localization/anti-weak localization effect and Shubnikov-de Haas oscillation directly reflect Berry's phase and valley degrees of freedom. With the decrease of dimension, the electron-electron correlation effect is significantly enhanced, which leads to the transport deviation from the traditional Drude model.

4.2. The transportation operation under field control is as follows

Gate voltage, magnetic field and light field are the key means to regulate low-dimensional quantum transport. Electrostatic gate control can continuously adjust the carrier concentration and Fermi level position, realize the transition from insulating state to metallic state, and induce superconductivity and associated insulating state in systems such as double-layer corner graphene [12]. Under the strong magnetic field, the 2D system enters the quantum Hall region, and the edge state transport shows no dissipative characteristics. However, in 1D/0D system, the magnetic field can remove the spin/valley degeneracy and modulate the Kondo resonance peak [13]. Light field driving opens up a new path for non-equilibrium transport, and dynamically modifies the energy band structure through Floquet engineering to realize photo-induced topological phase transition or photon-assisted tunneling, which provides the foundation for ultrafast quantum devices.

4.3. Topology and spin-dependent transport

Protected edge state/surface state transport in topological materials is a hot research topic at present. In quantum spin Hall insulator, the spiral edge state is immune to nonmagnetic impurities, resulting in accurate quantized longitudinal conductance [14]. The magnetic topological insulator further introduces time reversal symmetry breaking to realize quantum anomalous Hall effect and axion insulation state [15]. In terms of spin transport, the spin-valley locking effect in 2D TMDs makes the valley polarized current selectively excited by circularly polarized light [16]; The neighbor effect in van der Waals heterojunction can effectively induce the spin-orbit coupling of Rashba, and realize the electronic control generation and detection of pure spin current.

4.4. Molecular scale transport and quantum interference

Quantum interference (QI) becomes the core mechanism of the dominant transport in the contact between monomolecular junctions and atoms. Constructive interference enhances transmission, while destructive interference can lead to a sharp drop in conductance by several orders of magnitude, forming a "quantum switch". This interference effect is highly sensitive to molecular configuration, anchoring groups and electrode coupling, which provides a theoretical basis for designing molecular rectifiers, thermoelectric converters and quantum sensors. In recent years, in situ control of the QI effect has been achieved based on mechanically controllable break junction (MCBJ) and scanning tunneling microscope break junction (STM-BJ) techniques [17], revealing the correction effects of vibrational mode decoherence and electron-phonon coupling on quantum transport. Table 3 below lists the comparison of quantum transport characteristics of different low-dimensional systems.

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Table 3. Comparison of quantum transport characteristics of different low-dimensional systems

System dimension	Typical materials/structures	Lead transportation mechanism	Feature scale	Typical experimental phenomena
0D	Semiconductor quantum dots, single-molecules	Coulomb blockade, Kondo effect	< 10 nm	Conductivity step, zero bias peak, charge stability diagram
1D	CNT, InAs nanowires	Luttinger liquid, ballistic transport	Diameter ranging from 1 to 10 nm	Quantum conductivity platform, power-law tunneling spectrum
2D	Graphene, MoS_2 TMDs	Weak (anti) localization, quantum Hall effect	Thickness<5 nm	SdH oscillation, semi integer quantum Hall, valley Hall
Topological state	HgTe QW, $MnBi_2$ Te_4	Chiral/helical edge state transport	Edge state width~nm	Quantum Hall conductance, non dissipative edge current
Molecular knot	Benzene derivatives, fullerenes	Quantum interference, resonant tunneling	Sub nanometer (~0.5-3 nm)	Conductivity bimodal/valley, switching ratio>10^3, thermoelectric enhancement

5. CONCLUSION

0D quantum dots exhibit artificial atomic characteristics through discrete energy levels and Coulomb blocking effects, and their conductance characteristics directly reflect the single electron tunneling process. 1D nanowires/carbon nanotubes realize ultra-high conductivity and Luttinger liquid behavior by virtue of Van Hof singularity and ballistic transport mechanism. 2D materials, such as graphene, rely on Dirac fermion and topological edge states to exhibit weak localization control and quantum Hall effect. Landauer-Büttiker formula and non-equilibrium Green's function method successfully explain the core phenomena such as quantum tunneling, Kondo resonance and topological protection transport, which provide universal tools for cross-scale simulation. External field control can induce superconducting phase transition, photoinduced topological phase transition and other new states of matter, and the quantum interference effect in molecular junctions opens up a new path for thermoelectric conversion and quantum sensing. Although the current research has made breakthrough progress, the theoretical modeling accuracy of strong correlation system, real-time observation of multi-body interaction and functional optimization of new heterojunction still face challenges. In the future, it is necessary to combine first-principles calculation and in-situ detection technology to deepen the understanding of the regulation mechanism of low-dimensional quantum systems and promote their transformation and application in spintronics, quantum information processing and energy storage.

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