

Chapter 2

Theoretical Background

The quantum conductance is one of the most famous novel properties of the single-molecule junction as a one-dimensional conductor. The dI/dV spectra of the single-molecule junction give basic information about the interaction between the transported electron and vibration of the molecule. This chapter presents the theoretical background of these novel physical phenomena of single-molecule junctions.

2.1 Electric States in One-Dimensional Conductor

One-dimensional conductors have different conductance states than three-dimensional conductors [1, 2]. Here, a one-dimensional conductor is considered to be on the nanoscale in the x and y directions but infinite in the z direction. The Schrödinger equation can be expressed as in Eq. (2.1).

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(R) \right] \varphi(R) = E\varphi(R) \quad (2.1)$$

Because the potential in the z direction is zero, the system can be described by a free electron model. The three-dimensional potential $V(R)$ can be described as $V(x, y)$. The wave function in the z direction can be described as $\varphi = \varphi(x, y)\exp(ik_z z)$, and the Schrödinger equation is expressed as in Eqs. (2.2) and (2.3).

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y) \right] \varphi(x, y)\exp(ik_z z) = E\varphi(x, y)\exp(ik_z z) \quad (2.2)$$

$$\left[\frac{\hbar^2 k_z^2}{2m} - \frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + V(x, y) \right] \varphi(x, y) \exp(ik_z z) = E \varphi(x, y) \exp(ik_z z) \quad (2.3)$$

The wave function is satisfied by Eq. (2.4).

$$\left[\frac{\hbar^2 k_z^2}{2m} \right] \exp(ik_z z) = E_z \exp(ik_z z) \quad (2.4)$$

Therefore, $E_z = \frac{\hbar^2 k_z^2}{2m}$ in the z direction. On the other hand, the wave function is satisfied by Eq. (2.5) in the x and y directions.

$$\left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + V(x, y) \right] \varphi(x, y) = E_{x,y} \varphi(x, y) \quad (2.5)$$

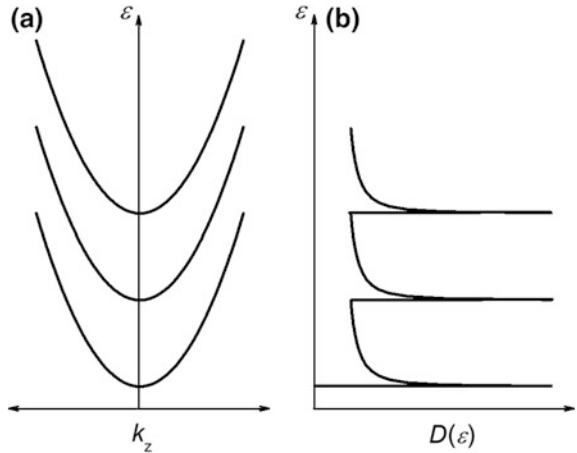
When we assume a rectangular conductor, $\varphi(x, y)$ and $E_{x,y}$ are the same as the eigen function and eigen energy, respectively, in quantum wells. Hence, the eigen energy of a one-dimensional conductor can be expressed as follows:

$$E = E_{i,j} + \frac{\hbar^2 k_z^2}{2m} \quad (2.6)$$

$$\phi = \exp(ik_z Z) \quad (2.7)$$

Figure 2.1a is the band distribution based on the Eq. (2.6) [1]. The parabola for each index notation i, j is called an electric subband. The density of states of the subband and D_{ij} is expressed as follows, and the density of states can be described as in Fig. 2.1b [1].

Fig. 2.1 Schematic representations of the **a** electronic states and **b** density of states of a one-dimensional conductor



$$D_{ij} = \frac{dN_{ij}}{dk} \frac{dk}{dE} \quad (2.8)$$

$$D_{ij} = \frac{4L}{\hbar v_{ij}} \quad (E > E_{ij}) \quad (2.9)$$

$$D_{ij} = 0 \quad (E < E_{ij}) \quad (2.10)$$

where v_{ij} is the velocity of the electron in the i, j subband. When there are different subbands, the subbands can be called “modes” and “channels.”

2.2 Electron Transport in Nano-Sized Conductor

The electron transport of an atomic-sized conductor is different from that of a bulk-sized conductor. In a bulk-sized conductor, the electron transport is diffusive, as shown in Fig. 2.2a. The electrons scatter at scattering points such as impurities and defects. The conductance of the bulk-sized conductor obeys Ohm’s law, and it is proportional to the area S and electrical conductivity σ , as shown in Eq. (2.11).

$$G = \sigma S/L \quad (2.11)$$

When the size of the conductor reaches the atomic scale, electron transport is influenced by the size of the conductor relative to the mean free path (l) and phase-coherence length (l_ϕ). The mean free path, which represents the distance traveled by an electron between collisions, is about 100 nm, whereas l_ϕ represents the distance within which the phase information is preserved. For gold, l_ϕ is on the scale of 1 μm . Therefore, the single-atom and single-molecule junctions discussed in this thesis are smaller than l and l_ϕ . In this region, electrons travel ballistically though the conductor, as shown in Fig. 2.2b.

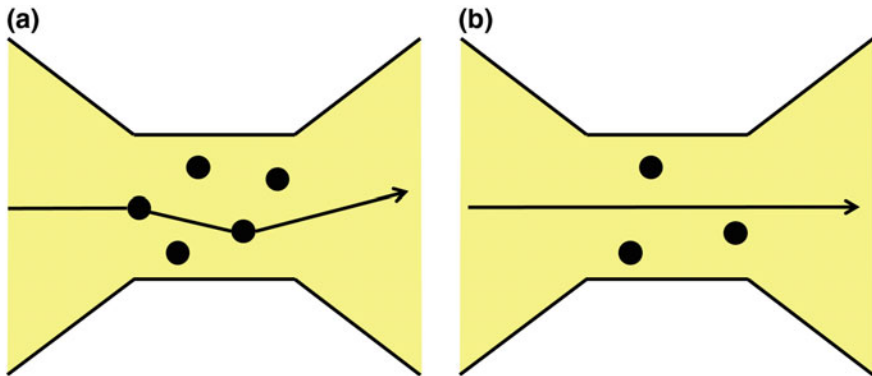


Fig. 2.2 Schematic diagram of **a** diffusive and **b** ballistic electron transport

2.3 Landauer–Büttiker Formula

Here, we consider electron transport through an atomic-sized conductor utilizing the scattering approach. In this approach, the sample works as a scattering point, which connects to the left (L) and right (R) electrodes over which the electron scattering is negligible, as shown in Fig. 2.3 [3]. The electrodes function as reservoirs of carriers, which is determined by the Fermi–Dirac distribution function. The Fermi–Dirac distribution function is described as follows:

$$f_\alpha = \frac{1}{\exp\left[\frac{E - \mu_\alpha}{k_B T_\alpha}\right] + 1} \quad (2.12)$$

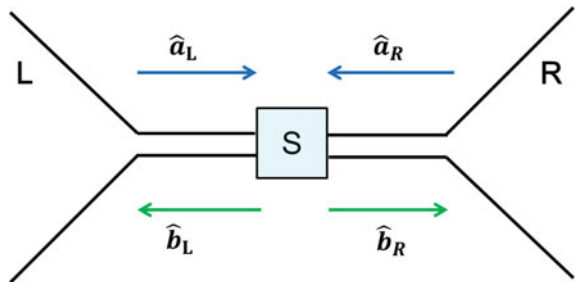
where the parameters μ_α and T_α represent the chemical potential and temperature, respectively, of the left and right electrodes, and k_B is the Boltzmann constant. As discussed in the previous section, the wave function can be expressed separately in the longitudinal and transverse directions, and its energy is expressed by Eq. (2.6). The electron transport can be separated into incoming and outgoing states depending on the sample for each electrode. In order to express the incoming and outgoing states, we introduced creation and annihilation operators. For the outgoing states, we expressed the creation and annihilation operators as $\hat{a}_{\alpha n}(E)$ and $\hat{a}_{\alpha n}^\dagger(E)$, respectively. For the incoming states, we expressed the operators as $\hat{b}_{\alpha n}(E)$, $\hat{b}_{\alpha n}^\dagger(E)$, respectively. The index n represents the quantum number to describe the quantum channels. The two operators were connected via the scattering matrix S :

$$\begin{pmatrix} \hat{b}_{L1}(E) \\ \vdots \\ \hat{b}_{RN_R}(E) \end{pmatrix} = S \begin{pmatrix} \hat{a}_{L1}(E) \\ \vdots \\ \hat{a}_{RN_R}(E) \end{pmatrix} \quad (2.13)$$

The scattering matrix S is described using the transmitting (t) and reflecting states (r) as follows:

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \quad (2.14)$$

Fig. 2.3 Schematic view of the scattering approach for two terminal conductors



The dimensions of each element are characterized by the quantum number of each electrode, which is related to the number of channels. The dimensions of each element are $N_L \times N_L$, $N_R \times N_R$, $N_R \times N_L$, and $N_L \times N_R$, for r , r' , t , and t' , respectively. In total, the dimensions of the scattering matrix are $(N_L + N_R) \times (N_L + N_R)$. The flux conservation and time-reverse symmetry lead to the unique unitary and symmetric character of the scattering matrix. The current operator in the left electrodes can be described using the field operator Ψ_L .

$$\hat{I}_L(z, t) = \frac{\hbar e}{2im} \int d\mathbf{r}_T \left[\hat{\Psi}_L^\dagger(\mathbf{r}, t) \frac{\partial}{\partial z} \hat{\Psi}_L(\mathbf{r}, t) - \left(\frac{\partial}{\partial z} \hat{\Psi}_L^\dagger(\mathbf{r}, t) \right) \hat{\Psi}_L(\mathbf{r}, t) \right] \quad (2.15)$$

$$\hat{\Psi}_L(\mathbf{r}, t) = \int dE e^{-iEt/\hbar} \sum_{n=1}^{N_L} \frac{\chi_{Ln}(\mathbf{r}_T)}{\sqrt{2\pi\hbar v_{Ln}(E)}} [\hat{a}_{Ln} e^{ik_{Ln}z} + \hat{b}_{Ln} e^{-ik_{Ln}z}] \quad (2.16)$$

$$\hat{\Psi}_L^\dagger(\mathbf{r}, t) = \int dE e^{\frac{iEt}{\hbar}} \sum_{n=1}^{N_L} \frac{\chi_{Ln}^*(\mathbf{r}_T)}{\sqrt{2\pi\hbar v_{Ln}(E)}} [\hat{a}_{Ln}^\dagger e^{-ik_{Ln}z} + \hat{b}_{Ln}^\dagger e^{ik_{Ln}z}] \quad (2.17)$$

$\mathbf{r}_T$ is the transverse coordination, and z is the coordination along the leads. $\chi_{Ln}(\mathbf{r}_T)$ are the transverse wave functions. Because the observable values do not change drastically, especially near the Fermi energy, we can neglect the energy dependence of the quantities. For the condition where the physical quantity does not depend on the energy, the current operator is expressed as follows:

$$\hat{I}_L(t) = \frac{e}{2\pi\hbar} \sum_n \int dE dE' e^{i(E-E')t/\hbar} [\hat{a}_{Ln}^\dagger(E') \hat{a}_{Ln}(E) - \hat{b}_{Ln}^\dagger(E') \hat{b}_{Ln}(E)]$$

where $\hat{n}_{Ln}^+(E)$ is the operator of the occupation number of the incident electrons in the left leads, $\hat{n}_{Ln}^-$ is the operator of the occupation number of the outgoing electrons in lead L in channel n , and $\hat{n}_{Ln}^+(E)$ and $\hat{n}_{Ln}^-(E)$ are expressed by Eqs. (2.19) and (2.20), respectively.

$$\hat{n}_{Ln}^+(E) = \hat{a}_{Ln}(E') \hat{a}_{Ln}^\dagger(E) \quad (2.19)$$

$$\hat{n}_{Ln}^-(E) = \hat{b}_{Ln}(E') \hat{b}_{Ln}^\dagger(E) \quad (2.20)$$

Now, $E' = \hbar\Omega + E$, and integrating over Ω yields:

$$\hat{I}_L(t) = \frac{e}{2\pi\hbar} \sum_n \int dE [\hat{n}_{Ln}^+(E, t) - \hat{n}_{Ln}^-(E, t)] \quad (2.21)$$

where $\hat{n}_{Ln}^\pm(E, t)$ are the time-dependent occupation numbers. Equation (2.21) shows that the current can be expressed as the difference in the occupation number in the electrodes. Equation (2.21) is then reexpressed using the scattering matrix S ,

$$\hat{I}_L(t) = \frac{e}{2\pi\hbar} \sum_{\alpha\beta} \sum_{mn} \int dE dE' e^{\frac{i(E-E')t}{\hbar}} \hat{a}_{\alpha m}^\dagger(E) A_{\alpha\beta}^{mn}(L; E, E') \hat{a}_{\beta n}(E') \quad (2.22)$$

$$A_{\alpha\beta}^{mn}(L; E, E') = \delta_{mn} \delta_{\alpha L} \delta_{\beta L} - \sum_k S_{L\alpha;mk}^\dagger(E) S_{L\beta;kn}(E') \quad (2.23)$$

Note that α and β represent the electrodes R and L, respectively. $S_{L\alpha;mk}(E)$ is the element of the scattering matrix that relates $\hat{b}_{Lm}(E)$ to $\hat{a}_{\alpha k}(E)$. At equilibrium, the mean square of the annihilation operator is

$$\langle \hat{a}_{\alpha m}^\dagger(E) \hat{a}_{\beta n}(E') \rangle = \delta_{\alpha\beta} \delta_{mn} \delta(E - E') f_\alpha(E) \quad (2.24)$$

The mean current in the junction is derived from Eq. (2.22):

$$\langle I_L \rangle = \frac{e}{2\pi\hbar} \int dE Tr \left[t^\dagger(E) t(E) \right] [f_L(E) - f_R(E)] \quad (2.25)$$

The matrix t is the off-diagonal block of the scattering matrix, and $t_{mn} = S_{RL;mn}$. At the limit of 0 K and a small voltage, the electrical conductance G is

$$G = \frac{e^2}{h} Tr \left[t^\dagger(E_F) t(E_F) \right] \quad (2.26)$$

The matrix $[t^\dagger(E) t(E)]$ can be diagonalized. The eigenvalues of $t^\dagger(E) t(E)$ yield the transmission probability, T_n , and the mean current and conductance are expressed as follows:

$$\langle I_L \rangle = \frac{e}{2\pi\hbar} \int T_n dE [f_L(E) - f_R(E)] \quad (2.27)$$

$$G = \frac{e^2}{h} \sum T_n \quad (2.28)$$

When we consider the spin degeneracy, the Landauer–Büttiker expression is derived as

$$G = \frac{2e^2}{h} \sum T_n \quad (2.29)$$

The conductance is expressed using only the transmission probability. Note that the conductance of the bulk metal depends on the temperature. The term $2e^2/h$ is referred to as the quantum unit and is expressed as G_0 , which has a conductance of about 77 μS or 13 $\text{k}\Omega$. If the transmission probability of all transmission channels is one, the conductance is an integer multiple value of G_0 .

2.4 Electron Transport in a Single-Molecule Junction

In the model proposed by Paulsson, the molecule in a molecular conductor behaves like a quantum dot [4]. We assume that the electron tunnels through double barriers [5], as shown in the upper panel of Fig. 2.4. The scattering matrix for barriers 1 and 2 are expressed as follows:

$$S_1 = \begin{pmatrix} r_1 & t'_1 \\ t_1 & r'_1 \end{pmatrix}, \quad S_2 = \begin{pmatrix} r_2 & t'_1 \\ t_2 & r'_1 \end{pmatrix} \quad (2.30)$$

Both S_1 and S_2 are unitary, and the amplitude A of the wave function is given by Eq. (2.31).

$$A = \frac{t_1 t_2 e^{ikW}}{1 - r_2 r'_1 e^{2ikW}} \quad (2.31)$$

W is the distance between two barriers, and k is the momentum of the electron. The transmission probability T_0 is given by the square of the amplitude.

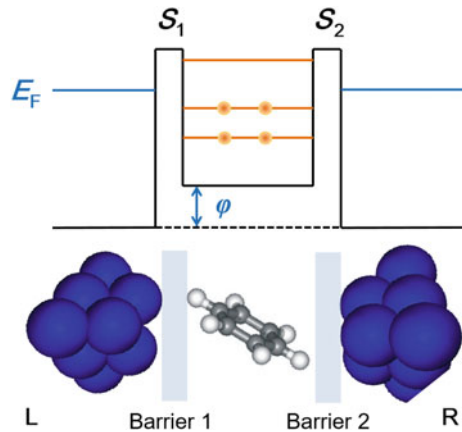
$$T_0 = \frac{T_1 T_2}{1 - 2\sqrt{R_1 R_2} \cos(2kW + \delta) + R_1 R_2} \quad (2.32)$$

T_γ and R_γ are the transmission and reflection at barriers 1 and 2, respectively, and δ is the declination of r_2 and r' . T_0 reaches a maximum at

$$2kW + \delta = 2\pi l \quad (l \text{ is an integer}) \quad (2.33)$$

Equations (2.32) and (2.33) imply that the energy in the quantum dot is discrete. When the energy of the incident electron is equal to the discrete energy level,

Fig. 2.4 Schematic energy diagram of the resonant-tunneling model with a double barrier (*top*) and schematic view of a single-molecule junction (*bottom*)



T_0 reaches a maximum at the resonance position. Now, T_1 and T_2 are small, and the resonant position shifts from $\varphi = \varphi_0$ to $\varphi = \varphi_0 + \delta$. The momentum k is expressed by $k = [2m(E + \varepsilon\varphi)/\hbar^2]^{1/2}$, and k shifts to $k + (\varepsilon/v_F\hbar)$. The transmission probability T_0 is expressed by

$$T_0 \approx \frac{T_1 T_2}{(1 - \sqrt{R_1 R_2})^2 + \sqrt{R_1 R_2} \left(\frac{2W\varepsilon}{\hbar v_F} \right)^2} \quad (2.34)$$

$$T_0 \approx \frac{\Gamma_1 \Gamma_2}{\varepsilon^2 + \frac{(\Gamma_1 + \Gamma_2)^2}{4}} \quad (2.35)$$

$$\Gamma_i = \frac{\hbar v_F T_i}{2R} \quad (2.36)$$

Here, Γ_i is the probability of the transition when an electron travels from the discrete level to the electron reservoir. The resonance is expressed by the Lorentz curve. The width Γ is expressed as the summation of the transition probabilities, Γ_1 and Γ_2 . Considering the single-transmission channel, the conductance value is given by

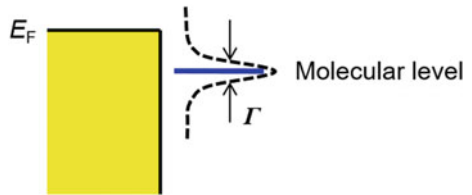
$$G = \frac{2e^2}{h} \frac{\Gamma_1 \Gamma_2}{\varepsilon^2 + (\Gamma_1 + \Gamma_2)^2/4} \quad (2.37)$$

In single-molecule junction systems, the double barriers are comparable to tunnel barriers between the molecule and electrodes. The discrete energy level is comparable to the energy level of the molecule. In the single-molecule junction, Γ_1 is described by the relaxation time as

$$\Gamma_i = e\hbar/\tau_i \quad (2.38)$$

Γ represents the line width of the energy level after interacting with metals [4], as shown in Fig. 2.5. When the electric coupling increases, the relaxation time decreases, leading to a higher Γ , which means that Γ represents the electric coupling between the metal and molecule [4]. The Fermi energy is located between the HOMO and LUMO. Because the energy level closest to the Fermi level plays an important role in electron transport, the discrete level that we refer to is either

Fig. 2.5 Schematic energy diagram of the metal electronic states and the molecular level



HOMO or LUMO. When the energy difference between the HOMO and E_F is smaller than that between the LUMO and E_F , the carrier is a hole. Otherwise, the carrier is an electron. Equation (2.37) indicates that the smaller energy difference between the molecule's orbital and E_F and the larger coupling Γ result in a large conductance value in the single-molecule junction.

Although the scattering approach explains physical quantities, such as the conductance, thermopower, and shot noise, expressing the properties of an individual single-molecule junction is difficult. In the scattering approach, it is difficult to preserve the intrinsic physical properties of a molecule and metal electrodes. In most cases, the transmission probability of the single-molecule junction is expressed using advanced and retarded nonequilibrium Green's function (NEGF) $G^{R/A}$.

$$T(E) = \text{Tr}[\Gamma_L(E)G^R(E)\Gamma_R(E)G^A(E)] \quad (2.39)$$

$$G^{R/A}(E) = \left[EI - H - \sum_L^{R/A}(E) - \sum_R^{R/A}(E) \right]^{-1} \quad (2.40)$$

where I and H are the unit matrix and Hamiltonian matrix of the molecule, respectively. Γ is expressed by the self-energy $\Sigma_{L(R)}^{R/A}$.

$$\Gamma_{L(R)} = i \left[\Sigma_{L(R)}^R - \Sigma_{L(R)}^A \right] \quad (2.41)$$

The real part of the self-energy yields the energy shift of the resonance position in Fig. 2.5, and the imaginary part indicates the broadening of the energy level. $\Gamma_{L(R)}$ represents the broadening function. For a weak coupling system, Green's function can be obtained from the zeroth Green's functions that are calculated separately for the electrodes and the molecule.

$$G_{RL}^{(0)R/A}(E) = \sum_k \frac{C_{R,k}C_{L,k}^*}{E - \varepsilon_k \pm i\eta} \quad (2.42)$$

where $C_{R,k}$, ε_k , and η represent the k th molecule's orbital coefficient at site R , the k th molecule's orbital energy, and the infinitesimal value, which is determined by the relationship between Green's function and the density of states (DOS). The term CC^* represents the orbital distribution of a molecule that is bridged between metal electrodes. The NEGF method has explained the conductance of graphene, single-molecule junctions, and many nano-sized conductors [6]. Equations (2.39)–(2.42) express the physical effects expressed by scattering models. The transmission probability derived by the Green's function explained the effects of the orbital alignments and the DOS of the metal electrodes.

2.5 Coupling Between Electron Transport and Vibration

2.5.1 Inelastic Electron Tunneling Spectroscopy

Evaluating the interface structure is important for understanding single-molecule junctions. Although scanning electron microscopy (SEM) can be used to successfully observe gold atomic contacts, the use of SEM is limited to observing fullerene molecules in studies on single-molecule junctions [7]. To identify a single molecule, Stipe et al. demonstrated the differential conductance measurement of an acetyl molecule on a Cu surface. The injected electron excites the vibration of the C–H stretching mode of the acetylene molecule [8]. The first derivative of the differential conductance dependence is called inelastic electron tunneling spectroscopy (IETS). In this section, the differential conductance behavior in an atomic-sized conductor is discussed. The electron–vibration coupling in the tunneling regime is described, as shown in Fig. 2.6. When $V < V_k$, the electron tunnels from the left electrode (L) to the right electrode (R). When the electron obtains sufficient energy to excite the vibration ($eV_k > h\omega$), the inelastic tunneling channel opens. The opening of this additional channel slightly increases the conductance of the junction. Therefore, the peak structure is observed in the d^2I/dV^2 spectrum in the tunneling regime.

In order for the tunneling electrons to excite vibration, the vibration should be coupled to the molecular orbital, which mainly contributes to the transport of electrons. The tunneling current that is enhanced by electron–vibration coupling is expressed as Eq. (2.43).

$$I_{\text{tunnel}} = \langle \Psi_{in} | M | \Psi_{fm} \rangle \quad (2.43)$$

Ψ_{in} and Ψ_{fm} are the initial and final states of inelastic scattering, respectively, and M represents the electron–vibration coupling matrix.

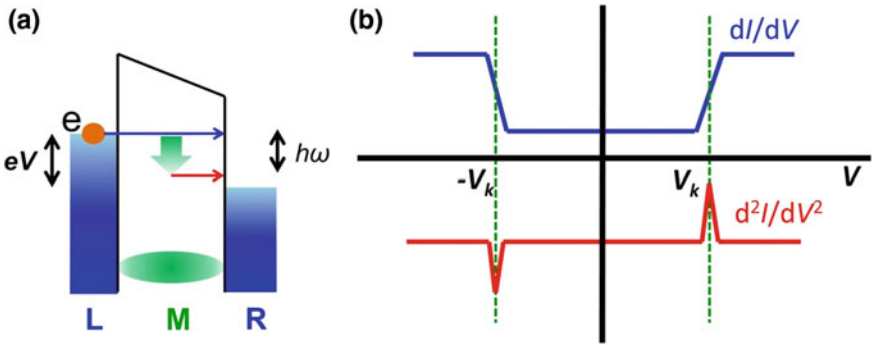


Fig. 2.6 **a** Schematic energy diagram of electron transport in the tunneling regime. **b** Typical dI/dV spectrum in the tunneling regime

2.5.2 Point-Contact Spectroscopy

In the case of nano-sized conductors with ballistic electron transport, measuring the dI/dV spectrum is called point-contact spectroscopy (PCS). In the ballistic transport regime, energy dispersion is described using a free electron model, as shown in Fig. 2.7a. In the ballistic regime, an electron occupies the states having momentum from $-k_z$ to $+k_z$ without a bias voltage. Note that k_z is the momentum in the direction parallel to the atomic junction. At a bias voltage of V_k , the electron obtains sufficient energy to excite the vibrational mode. Then, the electron transfers from the occupied states with a momentum of k_z to the unoccupied states with a momentum of $-k_z$, which indicates that electrons are backscattered, leading to a reduction in the conductance value. Therefore, a dip is observed at the vibrational energy in the d^2I/dV^2 spectrum in the ballistic regime, as shown in Fig. 2.7b.

2.5.3 d^2I/dV^2 Spectrum Behavior

In a realistic single-molecule junction, the differential conductance spectrum behavior is governed by the transmission probability T , where we assume a single

Fig. 2.7 **a** Energy dispersion in the ballistic regime.
b Typical dI/dV and d^2I/dV^2 spectra in the ballistic regime

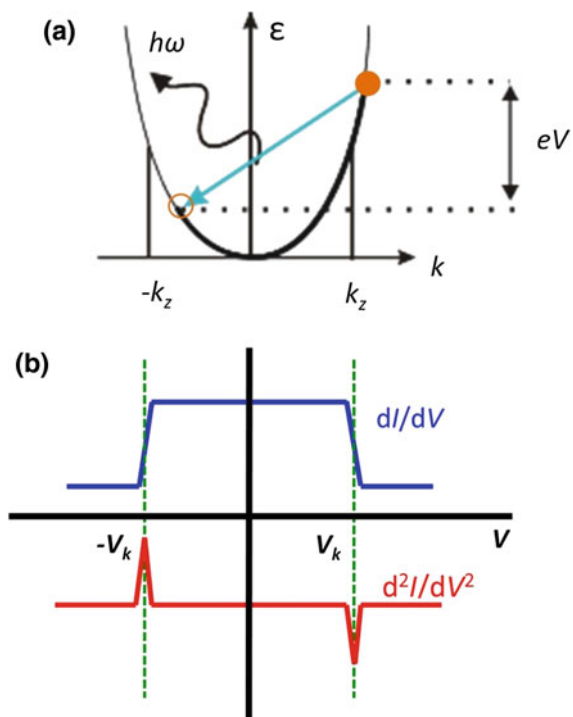
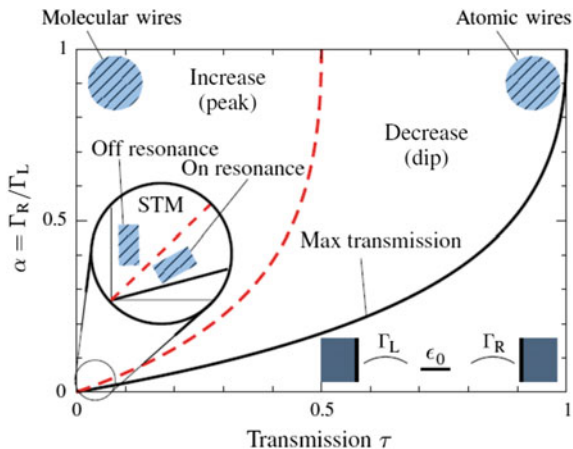


Fig. 2.8 d^2I/dV^2 spectrum behavior depending on the symmetry and transmission [10]. Reprinted with permission from Ref. [10]. Copyright 2008 by the American Physical Society



channel. The scattering approach also explains the limited understanding of the dI/dV spectrum behavior. In the ballistic regime, the ongoing states are fully occupied because almost all electrons travel from the left electrode to the right electrode. At V_k , the only states to which the electrons can transfer are the unoccupied incoming states, leading to a reduction of the conductance. On the other hand, in the tunneling regime, almost all electrons are reflected, and the incoming states are occupied. At V_k , the only states to which electrons can transfer are unoccupied outgoing states, leading to an increase in the conductance value. Paulsson et al. explained the d^2I/dV^2 spectrum behavior depending on the symmetricity (α) of the junction and transmission [9, 10], as shown in Fig. 2.8. When the junction is symmetric ($\alpha = 1$), the dI/dV response behavior changes from a peak to a dip at $T = 0.5$. This theory was experimentally verified with H_2O and 1,4-benzenedithiol molecules, both of which have single channels [11, 12].

The dI/dV spectrum also shows a characteristic shape when the tunneling electron induces the elementary process of a reaction triggered by the vibration excitation [13–16]. When the vibration coordination is the same as the reaction coordination, the reaction is induced by vibration with a higher energy than the reaction barrier. The hydrogen dissociation reaction of the trans-2-butene molecule on Pd(110) has been observed [14]. When the vibration coordination is not equal to the reaction coordination, the reaction is induced by the coupling between tunneling electrons and vibrational modes along the reaction coordination. In this mechanism, the CO molecule diffuses on the Cu substrate by the injection of the tunneling electrodes [15]. In a single-molecule junction, the transition between two meta-stable structures is observed by the injection of the tunneling electrons, thus exhibiting a peak structure in the dI/dV spectrum.

When a magnetic impurity exists on the nano-contacts, a peak or dip has been reported at $V = 0$, which is due to the Kondo effect. The Kondo effect is explained in terms of the many-body scattering problem. In a metallic atomic contact, this zero bias anomaly is also observed for Pt atomic junctions.

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Single-Molecule Junctions

A Focus on the Metal-Molecule Interface

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