

Quantum Tunneling from Giaever Junctions to Scanning Tunneling Microscopy

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Abstract

Quantum tunneling allows electrons to pass through a classically forbidden region. This effect can help us to research the electronic structure of materials. This paper examines how Giaever tunneling works and how to measure the energy gap and DOS. It then shows how these theories work in STM. This paper discusses the rectangular barrier model, the Bardeen–Giaever current theory, the Fermi occupation, and the superconducting DOS. It connects these theories to the Tersoff–Hamann STM model under particular assumptions. This paper derives how Giaever's tunneling current is determined by the DOS, the occupation window, and the tunneling matrix element. The transmission coefficient obeys $T \propto e^{(-2\kappa a)}$ and STM extended the theory into local density of states (LDOS). Giaever spectroscopy measures an area-averaged superconducting DOS, whereas STM measures spatially resolved LDOS; each model is valid only under its stated assumptions.

Keywords

quantum tunneling, scanning tunneling microscopy, Giaever junctions, Bardeen–Giaever current theory

1. Introduction

Classically, an electron with energy E cannot pass through a barrier with potential energy U , where $U > E$. In quantum mechanics, the electron has a probability to pass through the classical forbidden area, and the transmission coefficient is exponentially sensitive to the width and relative height $U-E$ of the barrier. This effect is known as quantum tunneling [1].

To investigate this effect, Giaever used two electrodes separated by a thin insulator. At cryogenic temperature, a low-bias I – V curve across the gap scale uses the tunnelling current and $\frac{dI}{dV}$ to identify the quasiparticle threshold and estimate the superconducting density of states (DOS). The key contributions were therefore the verification of the superconducting energy gap and the development of tunneling spectroscopy [2,3].

The purpose of this article is to investigate how the barrier controls the transition rate, how DOS and Fermi occupation affect the tunneling current and how Giaever's experiment can measure the energy gap. Finally, the article considers how these theories are used in scanning tunneling microscopy (STM).

2. Quantum Tunneling Through a Rectangular Barrier

2.1 Classical and Quantum Descriptions

Giaever measured a tunneling current through a planar metal–oxide–metal junction, even though this classically forbidden process crosses an insulating barrier [2,3].

In classical mechanics, the energy E of the electron in a potential $U(z)$ is defined as $\frac{p^2}{2m} + U(z) = E$, where p and m are the momentum and mass of the particle respectively. From this equation, when $U(x)$ is greater than E , the kinetic energy will be less than 0, so the particle has zero probability of passing a barrier with $U(z) > E$.

In quantum mechanics, the electron follows the Schrödinger wave function: $-\frac{\hbar^2}{2m} \frac{d^2\psi(z)}{dz^2} + U(z)\psi(z) = E\psi(z)$

The electron has a nonzero probability of passing through a barrier even if its energy is lower than the barrier [1].

For $E < U$ $\psi(z) = \psi(0)e^{-\kappa z}$

$$\kappa = \frac{\sqrt{2m(U-E)}}{\hbar}$$

This equation has two solutions which are $\psi(z) = \psi(0)e^{-\kappa z}$, decaying in the z direction and $\psi(z) = \psi(0)e^{\kappa z}$, decaying in the $-z$ direction. Both terms are retained because continuity at the two interfaces jointly determines the transmitted amplitude.

To be more specific, when $E < V_0$, most waves reflect and some pass through the barrier with their wavefunction amplitudes dropping exponentially with distance inside the barrier [1].

$$\frac{|\psi(z)|^2}{|\psi(0)|^2} = e^{-2\kappa z} \quad \kappa = \frac{\sqrt{2m(U-E)}}{\hbar}$$

The first relation gives the probability-density attenuation inside the barrier; T denotes the complete barrier transmission coefficient.

T depends mainly on the decay constant κ and the barrier width a . Here U is the barrier potential energy, E is the incident-electron energy, and m is the electron mass. A decrease in κ or an increase in κ increases the transmission probability [1].

2.2 Rectangular-Barrier Transmission

The system is divided into three regions, where the first region contains the incident and reflected waves with wave functions $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$. A is the incident amplitude and B is the reflected amplitude. In region II, $\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}$ the evanescent wave function is given by two independent exponential terms that are to make sure the gradient and value of the wave functions can match at the two interfaces of the single barrier. In region III, there is a transmitted wave with wave function $\psi_{III}(x) = Fe^{ikx}$, where F is the transmitted amplitude.

The boundaries of the barrier are at $x = 0$ and $x = a$ respectively. The four boundary conditions are:

$$\begin{cases} \psi_I(0) = \psi_{II}(0) \\ \psi_I'(0) = \psi_{II}'(0) \\ \psi_{II}(a) = \psi_{III}(a) \\ \psi_{II}'(a) = \psi_{III}'(a) \end{cases}$$

Since the wave functions and the gradients of the wave functions must be continuous at the two interfaces at $x = 0$ and $x = a$, the above equations must be met.

$T = \left[1 + \frac{V_0^2 \sinh^2(\kappa a)}{4E(V_0 - E)}\right]^{-1}$ This is the exact rectangular-barrier result. For a thick or high barrier, when $\kappa a \gg 1$, $\sinh^2(\kappa a) \approx \frac{e^{2\kappa a}}{4}$ [1].

the result reduces to $T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa a}$. When only a changes, the trend of the transmission coefficient is determined by $T \propto e^{-2\kappa a}$ [1].

The result for a single electron must be summed to obtain the junction's total current.

3. Tunnelling Current in the Bardeen-Giaever Framework

3.1 Bias Window and Transition Rate

Without an external voltage, the net tunneling current would be zero, since the currents in the two directions are equal. When we apply a bias voltage V , a net tunneling current occurs between states in electrode 1 and electrode 2 with energies between $E_F - eV$ and E_F . The current would be proportional to the bias voltage applied provided that $e|V| \ll \phi$, tunnelling is elastic, and the DOS and $|M|^2$ are about constant over the energy window [1].

In many-particle states of the system, we can't keep using the single-state transmission coefficient; we need to sum up occupied and empty states together to get the current. We could use the Bardeen matrix element $M_{\mu\nu}$ [4].

$$\Gamma_i = \frac{2\pi}{\hbar} |M_{if}|^2 \rho_f(E_i) \quad [4]$$

The transition rate is given by the above equation, where M is the matrix element and ρ_f is the density of the final states per unit energy. From the equation $\kappa = \frac{\sqrt{2m(U-E)}}{\hbar}$, $|\Delta\kappa|a \ll 1$ when there is a small change of energy. The wave function in the barrier region can be approximated as the same. Therefore it is reasonable to assume M is about a constant for $\Delta E \ll U - E$. We further assume that in the superconducting and normal states, M is approximately the same [4,5].

Therefore, from the equation, when M is assumed to be a constant, density of states in energy will be the factor affecting the transition rate $\Gamma_i \propto \rho_f(E_i)$ [4].

3.2 Net Current and Density of States

The following equation gives the net tunneling current

$$I(V) \propto \int_{-\infty}^{\infty} |M(E, V)|^2 \rho_1(E) \rho_2(E + eV) [f(E) - f(E + eV)] dE$$

where ρ_1 and ρ_2 are the two densities of states, $|M(E, V)|^2$ is the coupling weight, and $f(E) - f(E + eV)$ is the Fermi-function difference selecting occupied initial and empty final states [1,4].

At low temperature and low bias, the net tunnelling current is dominated by states near E_F . If the DOS and matrix element vary little across the narrow bias window, the equation becomes $I(V) \approx G(0)V$. $I \approx \frac{2\pi e^2 V}{\hbar} |M|^2 \rho_{\text{probe}}(E_F) \rho_{\text{surface}}(E_F)$. More generally, at low temperature with a slowly varying matrix element and tip DOS, dI/dV follows the sample DOS [4].

3.3 Bardeen Matrix Element

$$M_{\mu\nu} = -\frac{\hbar^2}{2m} \int_S (\psi_\mu^* \nabla \psi_\nu - \psi_\nu \nabla \psi_\mu^*) \cdot d\mathbf{S}$$

$M_{\mu\nu}$ is the matrix element between two states ψ_μ and ψ_ν . $|M_{\mu\nu}|$ represents the strength of the tunneling. $M_{\mu\nu}$ depends on the wave functions in the barrier and $\nabla\psi$, the gradient of which the wave function is changing relative to space. S is the integration surface. It is an imaginary surface that is completely in a vacuum or an

insulating barrier. When the tails of the Schrödinger functions are equal and the elastic equal-energy states satisfy the same local Schrödinger equation in the barrier, $M_{\mu\nu}$ is independent of the position of the integration surface because Bardeen transition-current flux is conserved [4].

$\kappa = \frac{\sqrt{2m(U-E)}}{\hbar}$; $\psi(d) \propto e^{-\kappa d}$ From the equations, when the barrier width d or the barrier height increases, ψ decreases. As a result $|M_{\mu\nu}|$ and $|M_{\mu\nu}|^2$ will decrease. It means that when the barrier width or height increases, wave overlap weakens and the transition rate decreases, resulting in less tunneling with fixed DOS [4].

4. Superconducting Density of States and Giaever Spectroscopy

4.1 Quasiparticles and Superconducting Density of States

$E = \sqrt{\epsilon^2 + \Delta^2}$, where E is the superconducting quasiparticle energy, ϵ is the energy of the electron in the normal state relative to the Fermi level and Δ is the superconducting energy-gap parameter.

In the superconducting state, electrons with energy near the Fermi level form Cooper pairs. Cooper pairing changes the quasiparticle excitation spectrum and causes an energy gap Δ . When $\epsilon = 0$, $E = \Delta$. This means Δ also indicates the minimum energy to create a quasiparticle excitation [4].

$$\rho_s(E) = \rho_n(E_F) \text{Re} \left[\frac{|E|}{\sqrt{E^2 - \Delta^2}} \right]$$

When $|E| < \Delta$, there is no corresponding DOS. When $|E| > \Delta$, DOS is calculated by the above equation and DOS is larger when $|E|$ is closer to Δ [4].

Because $\Delta \ll U - E_F$ and κ changes only slightly, the wave-function tails are roughly the same. Therefore, $M_{SC} \approx M_N$ [4,5].

Since $\frac{dI}{dV} \propto \rho_s(eV)$ the difference of tunneling current in superconducting states and normal states is mainly determined by the density of states in energy. When $|eV| < \Delta \Rightarrow I_{qp} = 0$, there's no available superconducting quasiparticle DOS, the tunneling effect is restricted. When $|eV_{th}| = \Delta$ DOS increases drastically. Therefore, the current rises sharply and the I-V curve can indicate the energy gap [2-4].

4.2 Junction Thresholds and Thermal Broadening

$$I(V) \propto \int |M(E, V)|^2 \rho_1(E) \rho_2(E + eV) [f(E) - f(E + eV)] dE$$

$$f(E; \mu, T) = \frac{1}{\exp \left[\frac{E - \mu}{k_B T} \right] + 1}$$

The current equation at low bias only indicates whether a corresponding state is possible. The Fermi function can determine whether the initial and final states are occupied or empty respectively. $|M|^2$ indicates the coupling strength through the barrier [1,4].

There are three types of junctions: normal-metal-insulator-normal-metal (N-I-N), superconductor-insulator-superconductor (S-I-S), and normal-metal-insulator-superconductor (N-I-S). At $T=0$ for single-quasiparticle tunneling. For N-I-N, there is no quasiparticle gap threshold. For N-I-S, there is a threshold $|eV_{th}|=\Delta$. For S-I-S, the threshold is $|eV_{th}|=\Delta_1+\Delta_2$ [2-4].

When the temperature is zero, in each electrode, electrons with energy below E_F are occupied, above E_F are empty. Therefore, the Fermi function exhibits a large step, and the occupation window has clear boundaries [1].

At finite temperature, over an energy range of order $k_B T$, electrons with energy above E_F start to have occupied states and below E_F start to have empty states. Therefore, thermal quasiparticles produce subgap current and the gap features are broadened, which means the occupation window is vaguer; the sharp current

onset is rounded and coherence peaks are widened. Therefore, the energy gap is harder to identify. Here, we discuss quasiparticle tunneling only; the Josephson pair current is not involved in the paper [1].

5. WKB Approximation for Real Barriers

5.1 WKB Transmission

$$T(E) \approx \exp \left[-2 \int_{z_1}^{z_2} \frac{\sqrt{2m[U(z) - E]}}{\hbar} dz \right]$$

This is the WKB expression, where $T(E)$ is the transmission coefficient. When $U(z)$ is a constant, the equation reduces to $T(E) \approx e^{-2\kappa d}$ [1].

In a real junction, bias tilts $U(z)$, so the WKB exponent changes with the barrier shape. Parabolic approximations simplify the calculation but have limited applicability [6,7].

5.2 Barrier Shape and Image-Force Effects

When there is an image force, $U(z) = U_0 - \frac{eVz}{d} + U_{\text{image}}(z)$ the effective thickness of the barrier will be reduced and the corners of the barriers will be rounded off. As a result, $U(z)$ and the WKB integral decrease, so $T(E)$ and the current increase. If the image-force effect is not considered, the current will be underestimated [6].

The current calculation is even more inaccurate when the effective barrier height ϕ is small. Because the correlations are poor, as the image force would have a greater influence. To obtain more accurate solutions, Simmons introduced a generalized tunneling-current formula using WKB for the true image-force potential [6].

6. Application to Scanning Tunnelling Microscopy

6.1 Constant-Current Imaging and the Tersoff-Hamann Model

$I \propto V e^{-2\kappa d}$ In the exponential equation, tunneling current is very sensitive to distance. For $\kappa \approx 1 \text{ \AA}^{-1}$, a $1 \text{ \AA}$ increase reduces the current by about e^{-2} [8,9].

The application of this is STM, which is used to display the structure of the sample by bringing the tip near the sample while applying a bias. One way for STM to work is the constant-current mode, in which the tip scans the x-y plane while adjusting the height z to maintain a constant current. The apparatus records the result and forms a contour map [8,9].

The low bias tunneling current has the equation

$$I(V) \approx G(0)V$$

$$G(0) = \frac{2\pi e^2}{\hbar} \sum_{\mu, \nu} |M_{\mu\nu}|^2 \delta(E_\mu - E_F) \delta(E_\nu - E_F) \quad [8].$$

Now we assume the tip is an ideal point probe which has a wave function arbitrarily localized around the tip position $\mathbf{r}_0$. This means $M_{\mu\nu} \propto \psi_\nu(\mathbf{r}_0)$ [8].

$$\rho_s(\mathbf{r}_0, E) = \sum_{\nu} |\psi_\nu(\mathbf{r}_0)|^2 \delta(E - E_\nu)$$

$$I(\mathbf{r}_0, V) \propto \int_0^{eV} \rho_s(\mathbf{r}_0, E_F + \varepsilon) d\varepsilon$$

DOS is the electron states of the whole sample per unit energy. In contrast, local density of states (LDOS), $\rho_s(\mathbf{r}_0, E)$ is the electron states of the sample near $\mathbf{r}_0$ per unit energy. The tunneling current through the tip indicates the LDOS near the Fermi level, and the two are proportional. Therefore, STM can form a contour map of constant surface LDOS [8,9].

However, an ideal point probe will be inaccurate for real tips. So Tersoff and Hamann assume the tip is locally spherical and that the work function of the tip equals the surface work function [8]. To evaluate M , we assume the tip has a wave function with an s-wave; this means for tips with other significant orbitals, the assumption should be changed [8]. So we still get the relation $I(\mathbf{r}_0, V) \propto V \rho_s(\mathbf{r}_0, E_F)$. This means the STM graph shows the electronic LDOS of the sample rather than a direct image [8].

6.2 Constant-Height Mode and Lateral Resolution

In constant-height mode, the tip height z is fixed and the tunnelling current $I(x, y)$ is recorded. It is faster than constant-current mode but less stable on rough surfaces, as the tip may crash; therefore, it is best suited to flat surfaces. The lateral resolution is estimated by $\Delta x_{\text{eff}} \approx \sqrt{(2 \text{ \AA})(R + d)}$ [9].

The effective lateral resolution is given by the above equation, where A is in $\text{\AA}$, R is the tip radius, and d is the vacuum distance. The limitation of this calculation is that the lateral resolution becomes poorer for large R and d [8].

7. Model Assumptions and Limitations

The one-dimensional piecewise-constant rectangular barrier has an exact analytic solution, but the model is too idealized. The Bardeen–Giaever model is only appropriate for weak coupling. WKB applies to slowly varying $U(z)$ relative to the local wavelength, but when $U(z)$ is changing rapidly relative to the local wavelength, or at turning points where $U(z)=E$, the solution will be inaccurate. The STM model can link current to LDOS but does not directly provide the geometric height of the sample [4,5,7,8,10].

8. Conclusion

In conclusion, in Giaever's apparatus, the thin insulating layer serves as a barrier, while a bias provides a range of available energy for tunneling. The Fermi factor determines the occupied and empty states, while the DOS determines the available states. This paper shows that tunneling current can be used to study the sample's electronic structure. Giaever tunneling spectroscopy measures the superconducting energy gap parameter and the area-averaged DOS, whereas STM measures the spatially resolved LDOS. Thus, the two methods use the same tunneling principle but address different material questions.

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Funding

This research received no external funding.

Conflicts of Interest

The authors declare no conflict of interest.

Acknowledgment

This paper is an output of the science project.

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