# Conductance images between two STM probes in graphene

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**Abstract**

The conductance image between two probes of scanning-tunneling-microscopy (STM) is calculated in a graphene within a tight-binding model and a realistic model for STM probes. A Kekulé-type pattern appears due to interference of states at K and K' points.

*Key words:* graphite, carbon nanotube, multi-probe STM, Kekulé-type pattern, quantum interference
*PACS:* 73.63.Fg, 68.37.Ef

## 1. Introduction

In an effective-mass approximation, an electron in a graphene is described by Weyl's equation for a massless neutrino [1]. Transport properties in such an exotic electronic structure are quite intriguing and studied theoretically, including universal minimum conductivity [2] and quantum correction to the conductivity [3]. It is known that scanning tunneling microscopy (STM) and spectroscopy (STS) are a powerful technique for directly viewing electronic wave functions at the atomic level. Quite recently multi-probe STM was developed [4]. The purpose of this paper is to explicitly visualize interference effects in two-probe STM images in graphene.

STM measurements have been conducted in order to observe the electronic wavefunctions in graphene [5, 6]. A characteristic $\sqrt{3}\times\sqrt{3}$ structure due to interference is observed near edge of a graphite [7, 8]. Electron transmission has been studied between two STM tips as leads which contact the nanotube via single carbon atoms [9], and associated orbital magnetic moments were discussed [10]. Recently, a Kekulé type pattern or $\sqrt{3}\times\sqrt{3}$ structure was shown to appear in two-probe STM images in carbon nanotubes due to interference of states at K and K' point except in special cases [11, 12]. In this paper, we calculate the conductance in a graphene and discuss robuster Kekulé pattern for tip position than that in carbon nanotubes.

## 2. Formulation

### *2.1. Preliminaries*

Figure 1 (a) shows the structure of two–dimensional (2D) graphite or graphene, two primitive translation vectors $\mathbf{a}$ and $\mathbf{b}$, and three vectors $\vec{\tau}_l$ ($l = 1, 2, 3$) connecting nearest-neighbor atoms. A unit cell contains two carbon atoms denoted as A (open circle) and B (closed circle). The origin of the coordinates is chosen at a B site, *i.e.*, a B site is given by $\mathbf{R}_B = n_a\mathbf{a}+n_b\mathbf{b}$ and an A site is $\mathbf{R}_A = n_a\mathbf{a}+n_b\mathbf{b}+\vec{\tau}$ with $n_a$ and $n_b$ being integers and $\vec{\tau}\equiv\vec{\tau}_1 = (\mathbf{a}+2\mathbf{b})/3$. In the coordinate system $(x, y)$, we have $\mathbf{a} = a(1, 0)$, $\mathbf{b} = a(1/2, \sqrt{3}/2)$, and $\vec{\tau} = a(0, 1/\sqrt{3})$, where $a = 0.246$ nm is the lattice constant. In the following we use a tight–binding model with a nearest–neighbor hopping integral $-\gamma_0$.

In a 2D graphite, two bands having approximately a linear dispersion cross the Fermi level at corner K and K' points of the first Brillouin zone. The wave vectors of the K and K' points are given by $\mathbf{K} = (2\pi/a)(1/3, 1/\sqrt{3})$ and $\mathbf{K}' = (2\pi/a)(2/3, 0)$. For states in the vicinity of the Fermi level $\varepsilon = 0$, the wavefunction is written as [1]

$$\psi_A(\mathbf{R}_A) = e^{i\mathbf{K}\cdot\mathbf{R}_A}F_A^K(\mathbf{R}_A) + e^{i\mathbf{K}'\cdot\mathbf{R}_A}F_A^{K'}(\mathbf{R}_A), \quad (1)$$

$$\psi_B(\mathbf{R}_B) = -\omega e^{i\mathbf{K}\cdot\mathbf{R}_B}F_B^K(\mathbf{R}_B) + e^{i\mathbf{K}'\cdot\mathbf{R}_B}F_B^{K'}(\mathbf{R}_B), \quad (2)$$

with $\omega = e^{2\pi i/3}$ in terms of the slowly–varying envelope functions $F_A^K$, $F_B^K$, $F_A^{K'}$, and $F_B^{K'}$. Then, in the vicinity of the K point, for example, they satisfy the $\mathbf{k}\cdot\mathbf{p}$ equation:

$$\gamma(\vec{\sigma}\cdot\hat{\mathbf{k}})\mathbf{F}^K(\mathbf{r}) = \varepsilon\mathbf{F}^K(\mathbf{r}), \quad (3)$$

$$\mathbf{F}^K(\mathbf{r}) = \begin{pmatrix} F_A^K(\mathbf{r}) \\ F_B^K(\mathbf{r}) \end{pmatrix}, \quad (4)$$

where $\gamma = \sqrt{3}a\gamma_0/2$ is the band parameter, $\hat{\mathbf{k}} = (\hat{k}_x, \hat{k}_y) = -i\vec{\nabla}$ is a wave vector operator, $\varepsilon$ is the energy, and $\sigma_x$ and $\sigma_y$ are the Pauli spin matrices.

Green's function is written as [13]

$$G_K = \begin{pmatrix} g_0 & g_1 \\ \bar{g}_1 & g_0 \end{pmatrix}, \quad G_{K'} = \begin{pmatrix} g_0 & \bar{g}_1 \\ g_1 & g_0 \end{pmatrix}, \quad (5)$$

where $\bar{g}_1(x, y) = g_1(x, -y)$ with elements calculated at $\varepsilon = 0$ and $r \gg a$ as

$$g_0 = 0, \quad (6)$$

$$g_1 = -i\frac{A}{2\pi}\frac{1}{r}e^{-i\varphi}. \quad (7)$$

Here $x = r\cos\varphi$, $y = r\sin\varphi$, and $A$ is a linear dimension of the system.

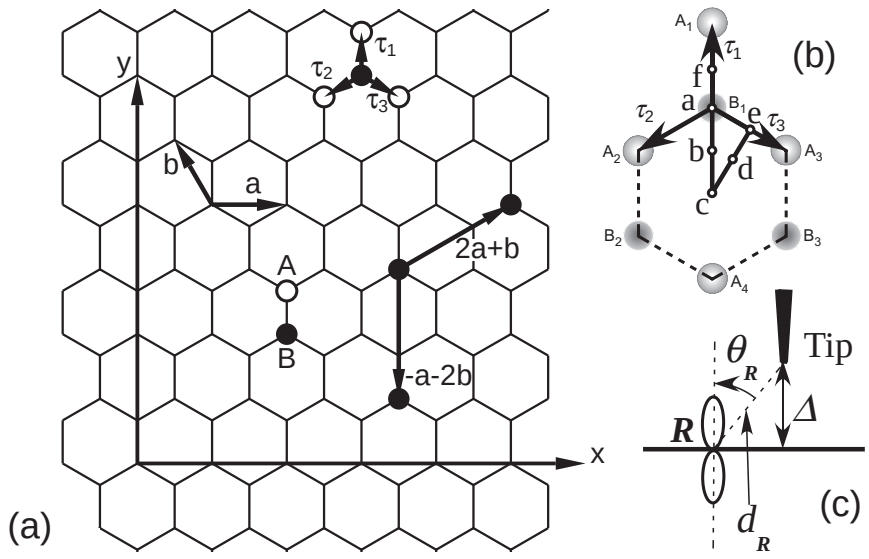


Figure 1: (a) Lattice structure of a two–dimensional graphite sheet. (b) The left STM-tip positions for which the STM image of the right tip is calculated. The actual coordinates are given in Table 1. (c) A model of the STM tip above a graphene with a $\pi$ orbital on a carbon atom at $\mathbf{R}$. $\Delta$ is the normal distance of the STM tip to the graphene.

### *2.2. Interference between K and K' Points*

We consider the conductance between two STM tips in a graphene. First, we consider propagating wave with $\varepsilon \approx 0$ injected from the B site $\mathbf{R}_B = 0$. We may approximately take the lowest order of the coupling between the STM tip and carbon atoms, because the coupling is usually very weak. Further, the wavefunction of the injected electron is decomposed into those at the K and K' point with the same amplitude. Then, Eq. (2) shows that the envelope functions outside the distance much longer than $a$ from the injection point $\mathbf{R}_B = 0$ become

$$\mathbf{F}^K(\mathbf{r}) = -\omega^{-1} G_K \frac{\delta}{\sqrt{2}A} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{8}$$

$$\mathbf{F}^{K'}(\mathbf{r}) = G_{K'} \frac{\delta}{\sqrt{2}A} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{9}$$

with $\delta$ being the amplitude. Upon substitution of the above into Eq. (2), we have

$$\begin{aligned} \psi_A(\mathbf{R_A}) &= -\frac{\mathrm{i}\delta}{2\pi\sqrt{2}} \frac{1}{r} (-\omega^{-1} \mathrm{e}^{-\mathrm{i}\varphi} \mathrm{e}^{\mathrm{i}\mathbf{K}\cdot\mathbf{R}_A} + \mathrm{e}^{\mathrm{i}\varphi} \mathrm{e}^{\mathrm{i}\mathbf{K}'\cdot\mathbf{R}_A}), \\ &= -\frac{\mathrm{i}\delta}{2\pi\sqrt{2}} \frac{1}{r} \omega\, \mathrm{e}^{\mathrm{i}(\theta+\varphi)} \Big[ 1 - \mathrm{e}^{-i(\theta+2\varphi)} \Big], \qquad (10) \\ \psi_B(\mathbf{R_B}) &= 0, \end{aligned}$$

with $\theta = 2\pi(n_a - 2n_b)/3$. The conductance between the STM probe at the origin and that at $\mathbf{R_A}$ is approximately proportional to the probability density

$$|\psi_A(\mathbf{R_A})|^2 = \left(\frac{\delta}{2\pi}\right)^2 \frac{1}{r^2} [1 - \cos(\theta + 2\varphi)]. \tag{11}$$

The conductance decays in proportion to the inverse of the square of the distance with oscillation. Around $\varphi \sim 0$ that is along $x$ axis, for example, conductance is finite $\propto (\delta/r)^2$ for $n_a - 2n_b = 3m \pm 1$ with an integer $m$ and vanishes for $n_a - 2n_b = 3m$.

The sites $\tilde{\mathbf{R}} = n_a\mathbf{a} + n_b\mathbf{b}$ satisfying $n_a - 2n_b = 3m$ with integer $m$ form a honeycomb lattice. Its basis vectors can be chosen as $\tilde{\mathbf{a}} = -\mathbf{a} - 2\mathbf{b}$ and $\tilde{\mathbf{b}} = 2\mathbf{a} + \mathbf{b}$ as shown in Fig. 1 (a), for example, and therefore the lattice constant is $\sqrt{3}a$ and the area of the unit cell is $3\Omega_0$ with $\Omega_0 = (\sqrt{3}/2)a^2$ being the area of the original honeycomb lattice spanned by the basis vectors $\mathbf{a}$ and $\mathbf{b}$. The maximum conductance is observed when two STM probes couple to atoms on this enlarged lattice for both A and B sublattices. This so-called Kekulé pattern is a result of the interference of traveling waves at the K and K' points as clearly shown in Eq. (10). The pattern also appears in the wavefunction around a single vacancy or edges [7, 8, 14].

### *2.3. Tip Model*

We consider a more realistic model of a graphene and an STM tip with coupling to several carbon atoms. The hopping integral between the tip $s$ atom and a $\pi$ orbital at $\mathbf{R}$ of the tube is given by $sp$ Slater–Koster form [15]:

$$t_{\mathbf{R}} = t_0 w_{\mathbf{R}} \exp\left(-\frac{d_{\mathbf{R}}}{\lambda}\right) \cos\theta_{\mathbf{R}}, \tag{12}$$

$$w_{\mathbf{R}} = \exp(-\alpha^2 d_{\mathbf{R}}^2) \Big[ \sum_{\mathbf{R}'} \exp(-\alpha^2 d_{\mathbf{R}'}^2) \Big]^{-1}, \tag{13}$$

where $d_{\mathbf{R}}$ is the distance between the tip atom and the carbon atom, $\theta_{\mathbf{R}}$ is the angle with the orientation of the $\pi$ orbital as shown in Fig. 1 (c). This model hopping integral with parameters $\lambda = 0.085$ nm, $\alpha^{-1} \approx 0.13$ nm, and $\Delta = 0.5$ nm has been

Table 1: The coordinates of the left STM tip shown in Fig. 1 (b) and the maximum values of the conductance, $G_{\max}$, used for plotting Figs. 2.

| | $3\Delta x/a$ | $\sqrt{3}\Delta y/a$ | $G_{\max}$ $(10^{-12}e^2/\pi\hbar)$ |
|---|---|---|---|
| (a) | 0 | 0 | 17.5 |
| (b) | 0 | -0.5 | 8.06 |
| (c) | 0 | -1 | $7.76 \times 10^{-4}$ |
| (d) | 0.4 | -0.6 | 7.33 |
| (e) | 0.75 | -0.25 | 11.5 |
| (f) | 0 | 0.5 | 11.5 |

introduced in previous works [15, 11]. The STM tip is modeled by a chain of *s*-like atoms with nearest neighbor hopping integral $-t$ and the Fermi energy being fixed at the center of the one-dimensional band.

Coupling between a graphene and STM probes is so weak that we may ignore mutual couplings and take only the lowest order of $t_{\mathbf{R}}$. We solve numerically Green's function $G_K$ and $G_{K'}$ on a lattice model of infinite graphene and calculate the transmission probability between two STM tips. In terms of the transmission probability $T$, the conductance $G$ is given by $G = (e^2/\pi\hbar)T$ using the Landauer formula. In actual calculations we choose fixed parameters $t_0/\gamma_0 = -10$, $t/\gamma_0 = 1$. Even if the Fermi wave length is shorter than the tip distance and thus the Fermi energy is away from zero energy, the calculated conductance images exhibit the same behavior except for an interference-like modulation due to the finite wave length.

## 3. Numerical Results

In the following, the left STM tip is fixed at several points marked by open circles in Fig. 1 (b) and the right tip is continuously swept over the wide region. The actual coordinates of the left tip are given in Table 1.

Figure 2 shows the conductance for varying the position of the right STM tip when the left tip is fixed at points 'a' to 'f' shown in Fig. 1 (b). The position of the left tip is denoted by an open circle, but its actual position is shifted by $(102, 0)a$ in the coordinate system $(x, y)$ shown in the Fig. 1 (a) and therefore is quite far from the right tip position.

When the left tip is on top of site $B_1$ denoted by 'a' in Fig. 2 (a), the conductance exhibits a clear Kekulé pattern and follows the simplified estimation presented in the previous section. In fact, the conductance is largest at A sites $\tilde{\mathbf{R}}_B + \tau_2$ and $\tilde{\mathbf{R}}_B + \tau_3$ related to the left-tip atom by the basis vectors $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{b}}$. Further, it vanishes at the other A and B sites. With the increase in the displacement 'b' to the hexagon center 'c' along the axis corresponding to (b) and (c), respectively, the similar image appears with the Kekulé pattern. At the hexagon center 'c', the image drastically changes and the maximum value of conductance becomes vanishingly small because of cancellation among couplings through several carbon atoms to propagating waves. Considering a states with uniform envelope function, which is mainly contribute to propagation at $\epsilon = 0$, we can show cancellation of their phases on three nearest-neighbor sites on the same sublattice with $1 + \omega + \omega^{-1} = 0$. With the increase in the deviation from the hexagon center, the image drastically changes at the center and varies continuously from (c) to (e). Around 'a' the images continuously vary from (e) to (f).

It has previously been demonstrated that in armchair nanotubes the Kekulé pattern disappears for special cases and original periodicity is recovered in the conductance images, due to the lack of interference between K and K' states [11, 12]. This is possible because there are only two modes propagating along the axis direction and the amplitude of one of the modes vanishes for a certain ratio of the injection from neighboring A and B sites. This also makes the STM image very sensitive to the left-tip position.

In graphene, on the other hand, there are propagating modes in all directions because of the two-dimensional nature and therefore the vanishing amplitude for a certain mode with a specific direction does not give rise to any visible effect. As a result, the STM images become robust for the change in the left-tip position. This allows us the observation of interference effects sensitive to intrinsic scatters such as ripples and point defects in graphene, avoiding ambiguity in the tip position.

## 4. Conclusions

We have calculated numerically the conductance between two STM probes in a graphene. The STM probes have been modeled with *sp* Slater-Koster hopping terms. It has been shown that a Kekulé pattern usually appears due to interference between propagating waves at K and K' points.

This work was supported in part by Grant-in-Aid for Scientific Research on Priority Area "Carbon Nanotube Nanoelectronics," by Grant-in-Aid for Scientific Research, by Global Center of Excellence Program at Tokyo Tech "Nanoscience and Quantum Physics" from Ministry of Education, Culture, Sports, Science and Technology Japan.

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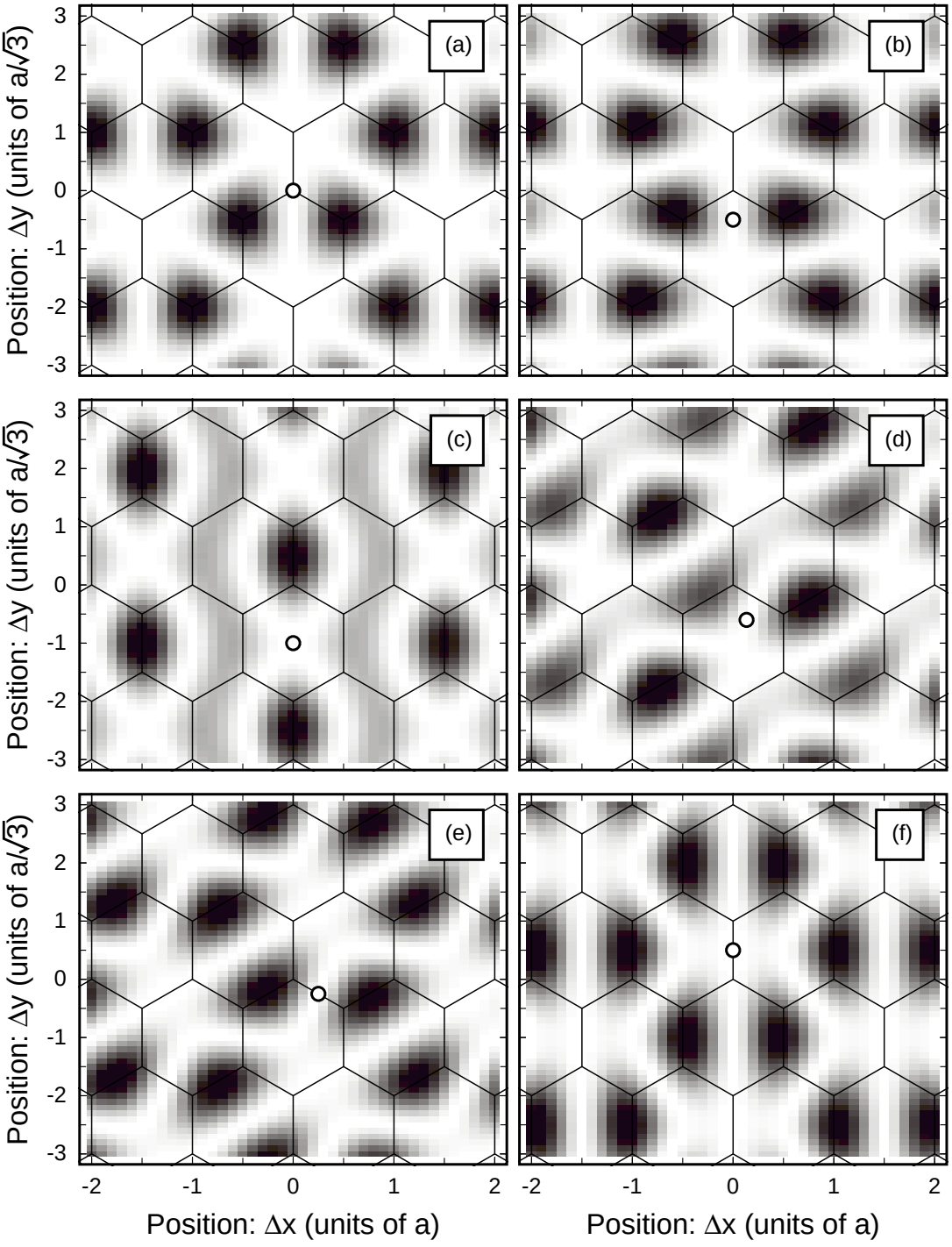


Figure 2: Calculated conductance as a function of right STM tip position for the left-tip position from 'a' to 'f' of Fig. 1 (b). The left STM tip is fixed above a position denoted by a open circle, but its actual position is at $(102, 0)a$ in the coordinate system and therefore is quite far from the right tip. The conductance is shown by the density in the maximum listed in a Table 1 as plot range.