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A MULTI-DIMENSIONAL TUNNELING THEORY WITH APPLICATION TO SCANNING TUNNELING MICROSCOPE(1)

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ABSTRACT

We have developed a formal general approach for evaluating the WKB wave function in a forbidden region of a non-separable potential in a three-dimensional space. The wave function is described by two sets of orthogonal wave-fronts, the equi-phase and equi-amplitude surfaces, or equivalently by two sets of paths defined to be normal to these surfaces respectively. We have extended a Huygens type construction to the forbidden region to obtain the multi-dimensional wave function. The construction determines the wave-fronts and the paths. It is found that the equations for the paths obtained from the construction are coupled to each other and do not reduce to a set of ordinary differential equations. However, if the incident wave is normal to the turning surface, the equations satisfied by the paths can be de-coupled. These equations are found to be equivalent to Newton's equations of motion for the inverted potential and energy. This characteristic has been used to calculate the current density distribution for an STM.

In this paper, we use the same approach to derive the expressions for the lateral resolutions and corrugations for a model STM.

1. Introduction

In many applications, exact analytical solutions of the Schrödinger equation are not available. Approximations are often needed to obtain the wave functions. A commonly used approach is the WKB method, which determines the asymptotic classical solution of the Schrödinger equation as \( \hbar \) goes to zero. In one dimension, the WKB wave function can be easily evaluated with the method in both the classically allowed and forbidden regions. In an allowed region in a multi-dimensional space, the WKB wave function can be written as an integral along the classical trajectory, which are determined by Newton's equations of motion [1]. Hence, the WKB method is also known as the semi-classical approximation.

In a forbidden region of a multi-dimensional space, the WKB wave function can be evaluated if the potential and the boundary conditions are separable [2]. For tunneling in a scanning tunneling microscope (STM), the potential is non-separable [3]. It is the purpose of this paper to present a method, similar to the Huygens construction, to determine the WKB wave function in the forbidden region.

The WKB wave function, in general, is described by two sets of orthogonal wave fronts, the equi-phase and equi-amplitude surfaces, or equivalently, by two sets of paths defined to be normal to these surfaces, respectively. We present in Section 2 a Huygens type construction for obtaining these wave fronts and paths. It is shown that the equations satisfied by the paths in the forbidden region are coupled. However, if the incident wave is normal to the turning surface, these path equations are de-coupled and are equivalent to Newton's equations of motion for the inverted potential and energy. The application to a model STM is presented in Section 3. The tunneling current density distribution is evaluated and the expressions for the lateral resolution and the corrugations are derived. These analyses are then compared to the results obtained by others. Section 4 is the conclusion of the paper.

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2. The WKB Wave function in a Multi-dimensional Space

By writing $\psi(\vec{r}) = \exp[iW(\vec{r})/\hbar]$, and substituting the expression into the Schrödinger equation, we obtain the lowest order approximation in $\hbar$ to the equation as

$$ [\nabla W(\vec{r})]^2 = 2m[E - V(\vec{r})] = \hbar^2[k(\vec{r})]^2. \tag{1} $$

In the allowed region, $W(\vec{r})$ is assumed to be real. Equation (1) can then be written as

$$ W(\vec{r}) = E(\vec{r}) = \hbar^2[k(\vec{r})]^2, \tag{2} $$

where $E$ is in the direction of $\nabla W(\vec{r})$. In the forbidden region, $W(\vec{r})$, in general, is complex, and can be replaced by two real quantities $W_R(\vec{r})$ and $W_I(\vec{r})$, i.e.,

$$ W(\vec{r}) = W_R(\vec{r}) + iW_I(\vec{r}). \tag{3} $$

Introducing two new wave vectors $k_R(\vec{r})$ and $k_I(\vec{r})$ such that

$$ W_R(\vec{r}) = \hbar k_R(\vec{r}), \tag{4a} $$
$$ W_I(\vec{r}) = \hbar k_I(\vec{r}). \tag{4b} $$

Using Eq. (3), (4a) and (4b), Eq. (1) becomes

$$ [k_R(\vec{r})]^2 - [k_I(\vec{r})]^2 = [k(\vec{r})]^2 = \frac{2m}{\hbar^2}[E - V(\vec{r})], \tag{5a} $$

$$ k_R(\vec{r}) \cdot k_I(\vec{r}) = 0. \tag{5b} $$

The WKB wave function $\exp[iW(\vec{r})/\hbar]$ can be determined by a Huygens type construction. Here only a brief outline of the method is presented. A more complete description of the method is presented in Reference 4.

To construct the wave function in the forbidden region, one starts with the turning surface, which separates the classically allowed region, labeled as region I, from the forbidden region, labeled as region II. The turning surface can be defined as the envelop of the classical trajectories. It is referred to as the caustic of the family of the trajectories. Since the WKB method fails at the caustic, other techniques are needed to obtain the wave function in the region. Using local separability, one finds that in region II near the caustic, the WKB wave function can be described by two wave vectors, $k_R(\vec{r})$ and $k_I(\vec{r})$, such that $\psi(\vec{r}) = \exp[i(k_R(\vec{r}) \cdot \vec{r} - k_I(\vec{r}) \cdot \vec{r})]$, with $k_R$ and $k_I$ being parallel and perpendicular respectively to the turning surface. To construct the wave function, we introduce two sets of surfaces, the constant phase ($W_R(\vec{r})$-constant) and constant amplitude ($W_I(\vec{r})$-constant) surfaces, and two sets of paths, the R-paths, being perpendicular to $W_R$-surfaces, and the I-paths, being perpendicular to $W_I$-surfaces. The wave function can then be written as $\psi(\vec{r}) = \exp[i(W_R(\vec{r}) - W_I(\vec{r}))/\hbar]$. It can be shown that $k_R(\vec{r})$ and $k_I(\vec{r})$ are parallel respectively to $W_R(\vec{r})$ and $W_I(\vec{r})$ surfaces, and are the vectors tangent to the R- and I-paths [4].

From Eq. (5), it follows that the two sets of paths are orthogonal. Similarly, the two sets of surfaces must be mutually perpendicular to each other. Since the solution near the caustic is known, and in particular the wave-vector $k_I$ is perpendicular to it, one may construct a $W_I$-surface near the caustic surface. Similar to the Huygens construction for optical rays, we construct the next $W_I$-surface, labeled as $W_I + \Delta W_I$, as follows: first choose a point, labeled as $M$, on the $W_I$-surface (see Fig. 1); the corresponding point, $M'$, on the $W_I + \Delta W_I$-surface is in the direction normal to $W_I$-surface at the point and a distance $\delta = \Delta W_I/\hbar k_I(\vec{r})$ away from point $M$, where $\delta$ is the arc length of the I-path. Since $k_I(\vec{r})$ is only known near the caustic, the next step is to determine $k_I(\vec{r})$ on the new surface, $W_I + \Delta W_I$.

However, it is easier to determine the change of $k_R(\vec{r})$ from point $M$ to point $M'$. This change is given by [4]

$$ \frac{\delta k_R(\vec{r})}{\delta \xi} = - k_R(\vec{r}) \frac{d\delta}{d\xi}, \tag{6} $$
Fig. 1. Schematic representation of two mutually orthogonal wave fronts, i.e., constant $W_R$ and $W_I$ surfaces.

where $\xi$ is the arc length of the $R$-path and $d\theta/d\xi$ is the curvature of the $R$-path in a two-dimensional space. In three-dimensions, it can be shown that $d\theta/d\xi$ is the curvature of the projected $R$-path onto a plane formed by $E_R$ and $E_I$. Consequently, the change of $k_I(\vec{r})$ in the direction of $E_I(\vec{r})$ is

$$\frac{\partial k_I(\vec{r})}{\partial \xi} = -\frac{k_I^2 + k^2}{k_I} \frac{d\theta}{d\xi} - \frac{k_I}{k_I} \frac{\partial k}{\partial \xi}.$$  

(7)

That is, the decaying wave vector $E_I(\vec{r})$ depends not only on the potential but also the bending of $R$-paths. It can be shown that if the $R$-paths on the $W_I$-surface is known, one can determine the $R$-paths on the $W_I + \Delta W_I$-surface[4]. The equations satisfied by the $R$- and $I$-paths can also be derived and are given as

$$k_I(\vec{r}) \frac{d^2x_I}{d\xi^2} - \frac{dx_I}{d\xi} \sum_j \frac{\partial k_I(\vec{r})}{\partial x_j} \frac{dx_I}{d\xi} = -\frac{\partial k_I(\vec{r})}{\partial x_I},$$  

(8a)

$$k_R(\vec{r}) \frac{d^2x_I}{d\xi^2} - \frac{dx_I}{d\xi} \sum_j \frac{\partial k_R(\vec{r})}{\partial x_j} \frac{dx_I}{d\xi} = -\frac{\partial k_R(\vec{r})}{\partial x_I}, \quad x_I = x,y,z.$$  

(8b)

These two equations are coupled to each other. However, if $E_R(\vec{r})$ vanishes, the equations are de-coupled. In fact, the equations for the $I$-paths can be derived from Newton’s equations of motion for the inverted potential and energy, i.e., $V = -V(r)$ and $E = -E$.

3. Application to STM

A model STM is shown in Fig. 2. For simplicity, the potential energy is assumed to be

$$V(r,z) = \begin{cases} V, & (r,z) \text{ in forbidden region,} \\ 0, & \text{otherwise.} \end{cases}$$  

(9)

The quantity of interest is the current density distribution, which is proportional to the transmission probability $D(E)$. If we assume that the incident wave is normal to the turning surface, then the wave function in the forbidden region is a purely decaying wave and can be described by $E_I(\vec{r})$. The trajectories can then be obtained from Newton’s equations of
Fig. 2. A model STM with no surface corrugation, where $R_T$ is the radius of the tip and $d$ is the distance from the tip to the sample.

motion. Since the potential energy is constant in the region, the trajectories are straight lines perpendicular to the hemispherical tip surface. The current density distribution can be easily evaluated using the WKB transmission probability:

$$j(r) \propto \exp\left(-2\kappa\left[\sqrt{(d+R_T)^2 + r^2} - R_T\right]\right),$$

(10)

where $\kappa^2 = \frac{2m}{\hbar^2} [V - E]$, $d$ is the tip-sample distance, and $R_T$ is the tip radius. Figure 3 is a plot of the current density $j$ as a function of cylindrical coordinate $r$ in the plane of the sample. It agrees with the results obtained by Lucas et al. [3].

Fig. 3. The current density distribution $j$ as a function of $r$. For the calculations, the following values are used: $V_m - E = 4.5eV$, $d = 5\text{Å}$, and $R_T = 3\text{Å}$.
In the above derivation, a perfectly flat planar sample surface is assumed, which is a good approximation only if the surface corrugation is negligible. A more realistic model is depicted in Fig. 4. If one assumes that the contribution only comes from one or a few most probable paths and their neighbors, the lateral resolution can easily be shown to be

\[ r_m = \frac{4ln2(R_T + R_S + d)}{\alpha} \]  \hspace{1cm} (11)

where \( R_S \) is the radius of the sample atoms. This agrees with the expressions given by others [5,6].

Fig. 4. A model STM with surface corrugation, where \( R_S \) is the radius of sample atoms and \( a \) is the spacing between the atoms.

The measured surface corrugation is the movement of the tip in the vertical direction under constant current. The condition for determining the amplitude of the corrugation \( \Delta \) is

\[ J|_{r=0} - J|_{r=a/2} \]

where \( r \) is the lateral displacement from the position where the tip is right above the surface atom and \( a \) is the separation of the surface atoms. If one assumes that the tunneling current is dominated by the most probable path (the path with the greatest probability for transmission through the barrier), it can be shown that the corrugation is

\[ \Delta = \sqrt{(R_T + R_S + d)^2} - R_T - R_S - d - \frac{ln2}{2\alpha} \]  \hspace{1cm} (13)

This result differs from the expression given by Tersoff and Hamann [5],

\[ \Delta_{TH} \propto \exp \left[-\frac{\pi^2(R_T+d)}{\kappa a^2}\right] \]  \hspace{1cm} (14)

However, the latter is for small corrugation, \( (\kappa \Delta_{TH} << 1) \).

4. Conclusions

We have developed a formal scheme, which may be regarded as an extension of Huygens construction, to construct the wave function in the forbidden region of a tunneling barrier using WKB approximation. It is shown that, in general, in a multi-dimensional space, the WKB approximation does not transform the quantum problem into a classical problem, i.e., the approximate wave function can not be obtained by solving Newton's equations of motion. Although one may still use two sets of paths, or trajectories, to describe the problem, these paths are coupled to each other. A special case is normal incidence, in which the two sets of paths are decoupled and are reduced to Newton's equations of motion. We have applied this property to the scanning tunneling microscope. The current density distribution and the expressions for the lateral resolution and the corrugation were derived.
References: