Surface state in quantum mechanics

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Figure 1 shows the 1D model potential for the surface state. We assume that atoms are ordered with the periodisity of a, and $z = 0$ is defined as the position of the topmost atom. The atoms form a periodic potential with the amplitude of $2V_1$, which is expressed as follows:

$$\begin{aligned} V(z) &= 2V_1 \cos \frac{2\pi}{a} z \\ &= V_1 \exp(igz) + V_1 \exp(-igz). \end{aligned} \tag{1}$$

Here, $g = 2\pi/a$. We assume that the atomic potential is effective at $z \leq a/2$, and the region with $z > a/2$ is a vacuum, where $V(z) = V_0$. The Schrödinger equation for the vacuum region is expressed as follows:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\psi(z) = E\psi(z) \tag{2}$$

$$\therefore \psi(z) = A \exp\left(-\frac{\sqrt{2m(E-V_0)}}{\hbar}\right) \tag{3}$$

Because the atomic lattice in the bulk is periodic, the wave function in the bulk should satisfy Broch's theorem as follows:

$$\psi_k(z) = \exp(ikz) \cdot u_k(z). \tag{4}$$

$u_k(z)$ is the periodic function for the lattice constant a. Thus, the Fourier transofrm of $u_k(z)$ is expressed as follows:

$$\begin{aligned} u_k(z) &= \sum_n a_n \exp(ingz) \\ &= \sum_n a_n \exp(iGz). \end{aligned} \tag{5}$$

Here, $G = ng = 2\pi n/a$. Therefore,

$$\begin{aligned} \psi_k(z) &= \exp(ikz) \cdot u_k(z) \\ &= \sum_n a_n \exp i(k+G)z. \end{aligned} \tag{6}$$

In a model called the "two-band model," we only consider the component with $n = 0, -1$.[1] Therefore, the bulk wave function in the two-band model is expressed as follows:

$$\psi(z) = a_0 \exp(ikz) + a_{-1} \exp[i(k-g)z]. \tag{7}$$

[1] In other words, we only consider the gap caused by the crossing of $n = 0$ and -1 states.

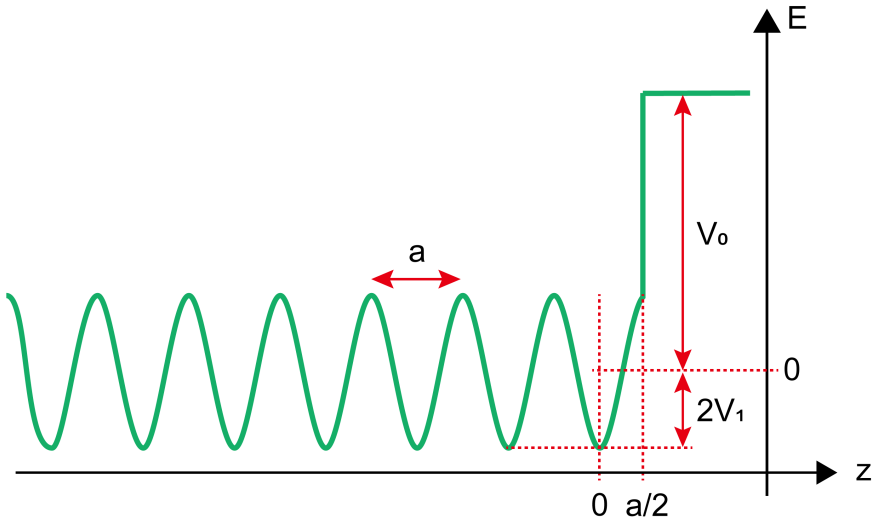

Figure 1: Model potential for considering the surface state.

Using eq.1 and eq.7, the Schrödinger equation of the bulk region is expressed as follows:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V_1 \exp igz + V_1 \exp(-igz)\right)(a_0 \exp(ikz) + a_{-1}\exp[i(k-g)z])$$
$$= E\,(a_0 \exp(ikz) + a_{-1}\exp[i(k-g)z]) \tag{8}$$
$$\therefore \left(\frac{\hbar^2 k^2}{2m}a_0 + V_1 a_{-1} - Ea_0\right)\exp(ikz) + \left(\frac{\hbar^2(k-g)^2}{2m}a_{-1} + V_1 a_0 - Ea_{-1}\right)\exp[i(k-g)z] = 0 \tag{9}$$

We ignored the terms except for $\exp(ikz)$ and $exp[i(k-g)z]$ because now we consider the two-band model. Equation 9 yields two equations:

$$\frac{\hbar^2 k^2}{2m}a_0 + V_1 a_{-1} - Ea_0 = 0 \tag{10}$$
$$\frac{\hbar^2(k-g)^2}{2m}a_{-1} + V_1 a_0 - Ea_{-1} = 0 \tag{11}$$

The matrix expression of these two equations is as follows:

$$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} - E & V_1 \\ V_1 & \frac{\hbar^2(k-g)^2}{2m} - E \end{pmatrix}\begin{pmatrix} a_0 \\ a_{-1} \end{pmatrix} = 0 \tag{12}$$

For a_0 and a_{-1} to have solutions, the determinant of the matrix should be zero, as follows:

$$\left(\frac{\hbar^2 k^2}{2m} - E\right)\left(\frac{\hbar^2(k-g)^2}{2m} - E\right) - V_1^2 = 0. \tag{13}$$

Using the replacement $k = \kappa + g/2$ and $b = \hbar^2/2m$, the solution is expressed as follows:

$$E = b\kappa^2 + b\left(\frac{g}{2}\right)^2 \pm \sqrt{b^2\kappa^2 g^2 + V_1^2} \tag{14}$$
$$a_{-1} = \frac{E - bk^2}{V_1}a_0. \tag{15}$$

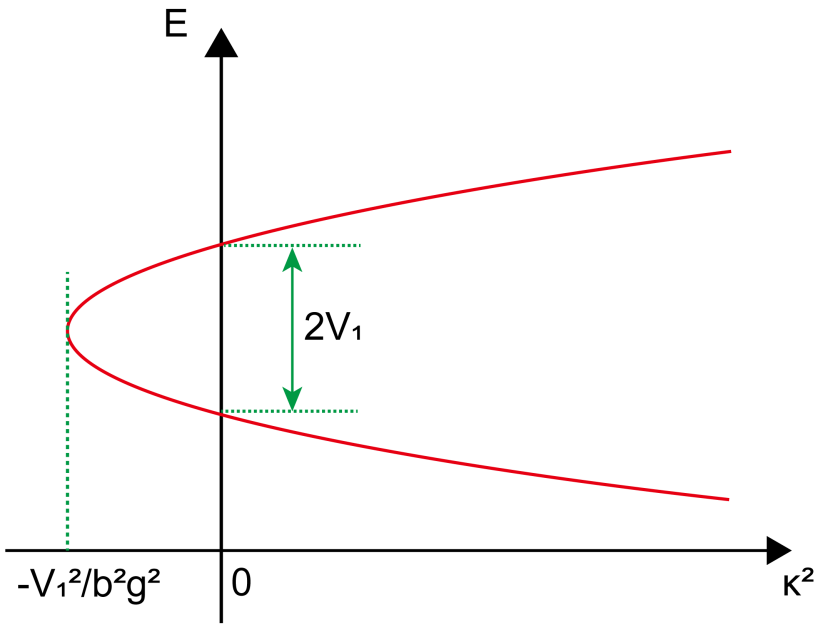

Figure 2: The relationship between the energy and κ^2.

Therefore, the wavefunction of the bulk part is expressed as follows:

$$\begin{aligned}\psi(z) &= a_0 \exp(ikz) + a_{-1} \exp[i(k-g)z] \\ &= a_0 \exp i\kappa z \left[\exp\left(i\frac{g}{2}z\right) + \frac{E-bk^2}{V_1}\exp\left(-i\frac{g}{2}\right)z\right]. \end{aligned} \tag{16}$$

Figure 2 is the schematic illustration of eq. 14. Energy level exists at $\kappa^2 \geq -V_1^2/b^2g^2$.

When $\kappa^2 \geq 0$, κ is a real value. Thus, the wave function in the bulk (eq. 16) oscillates without decay in the bulk. The energy states extend over the bulk, indicating that it corresponds to the bulk energy band, as schematically illustrated in Fig. 3. The two branches correspond to the upper and lower energy bands, and the bands are gapped by $2V_1$, corresponding to the bandgap.

When $\kappa^2 \leq 0$, κ is an imaginary value ($\kappa = \pm i\kappa'$, where κ' is an real value). Because if $\kappa = +i\kappa'$, the wave function diverges at $z \to \infty$, the solution is $\kappa = -i\kappa'$. In addition,

$$\left|\frac{E-bk^2}{V_1}\right| = \left|\frac{-b\kappa g \pm \sqrt{b^2\kappa^2g^2 + V_1^2}}{V_1}\right| \tag{17}$$

$$= \left|\frac{ib\kappa' g \pm \sqrt{V_1^2 - b^2\kappa'^2g^2}}{V_1}\right| \tag{18}$$

$$= 1. \tag{19}$$

It indicates that $\frac{E-bk^2}{V_1}$ is an imaginary value with the size of 1. Therefore, we can use the following expression:

$$\frac{E-bk^2}{V_1} = \exp(2i\delta). \tag{20}$$

The wave function in the bulk region is expressed as follows:

$$\psi(z) = a_0 \exp i\kappa z \left\{\exp i\frac{g}{2}z + \exp(2i\delta)\cdot\exp\left(-i\frac{g}{2}\right)z\right\} \tag{21}$$

$$= a_0 \exp i\delta \cdot \exp \kappa' z \cdot \cos\left(\frac{g}{2}z - \delta\right) \tag{22}$$

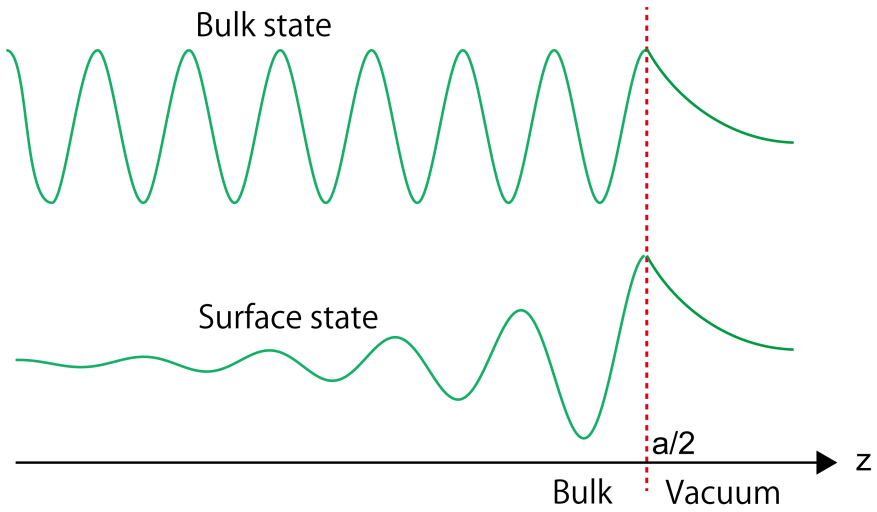

Figure 3: Schematic illustration of the bulk and surface state wave function.

Equation 22 not only oscillates but also decays for $z \to -\infty$. This wave function has the largest intensity at the surface, as shown in Fig. 3. Therefore, this state is called the surface state. As shown in Fig. 2, the energy of the surface state is located in the bulk bandgap. The phase factor δ is determined by the connection with the wave function in the vacuum (eq. 3).