

TUNNEL EFFECT IN METALLIC CRYSTALS

by

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According to our ordinary way of considering things, a fly enclosed in a well-formed bottle will never fly away unless it is strong enough to break the glass wall and escape. Newtonian mechanics predicts the same result, while wave mechanics tells us quite a different story. In wave mechanics, a particle of total energy E will penetrate a greater potential energy barrier, say V , and appear in the regions away from its originally bounded space according to certain quantum statistical laws. This phenomenon, named "the tunnel effect"⁽¹⁾, is particularly helpful in theoretical explanations of radioactive disintegration,⁽²⁾ chemical rate processes,⁽³⁾ metallic bonding and many other chemical facts. Under this title, we intend to formulate certain relations for barrier penetration probability with boundary conditions, and by them we are able to construct a correct intuitive picture of the phenomena concerning the metallic behavior.

I. Tunnel Effect With Boundary Conditions⁽⁴⁾

For particles of total energy E and potential energy V in one dimensional problems, Schroedinger equation of time independence is given :

Notes:

- (1) Many authors prefer to use barrier penetration or quantum mechanical leakage instead of tunnel effect.
- (2) Thorough treatments of α -decay, see, for example, M. Bcrn, *Atomic Physics*, G. E. Strechert & Co., 1951, pp. 202~206, 308.
- (3) See H. Eyring, J. Walter, G. E. Kimball, *Quantum Chemistry*, John Wiley & Sons, Inc., 1944, pp. 299~331.
- (4) Treatments in this section are restricted to one dimensional barrier problems. References see: a). D. Bohm, *Quantum Theory*, Prentice-Hall, Inc., 1951, pp. 238~240; b). H. Margenau, G. M. Murphy, *The Mathematics of Physics And Chemistry*, Van Nostrand Co. Inc., 1956, pp. 353~358; c). S. Golden, *Introduction to Theoretical Physical Chemistry*, Addison-Wesley Publishing Co. Inc., 1961, pp. 237~245.

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$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) = 0 \quad (1-1)$$

Taking energy equation in Hamiltonian form

$$E = \frac{p^2}{2m} + V \quad (1-2)$$

where p is momentum and m the mass of the particle. Solving for p , we have

$$p = \sqrt{2m(E - V)} \quad , \quad \text{with } E > V \quad (1-3)$$

and
$$p = i\sqrt{2m(V - E)} \quad , \quad \text{with } E < V \quad (1-4)$$

The prototype wave function and hence the solution of the differential equation (1-1) is given as:

$$\psi = A e^{i\kappa x} + B e^{-i\kappa x} \quad (1-5)$$

where
$$\kappa = \sqrt{2m(E - V)} / \hbar \quad , \quad \text{with } E > V \quad (1-6)$$

and
$$\kappa = i\sqrt{2m(V - E)} / \hbar \quad , \quad \text{with } E < V \quad (1-7)$$

A and B are two arbitrary constants.

Now let us first construct a barrier potential of the form as shown in Figure-1.

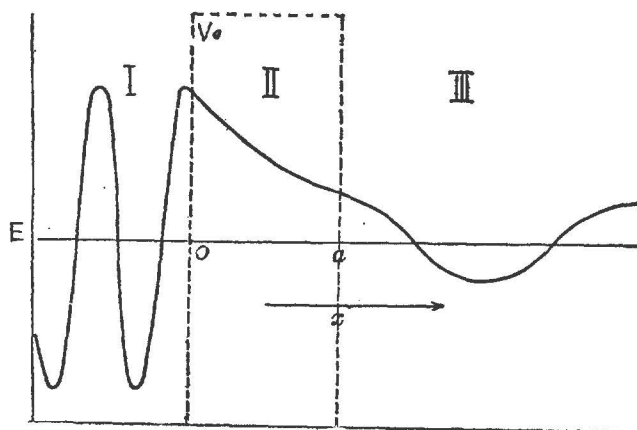


Fig. 1. Barrier penetration of particles

This potential is

$$\begin{aligned} V(x) &= V_0 \quad , \quad \text{for } 0 \leq x \leq a \\ V(x) &= 0 \quad , \quad \text{for } -\infty < x \leq 0 \text{ and } \infty > x \geq a \end{aligned} \quad (1-8)$$

where $V_0 \gg E$.

Notes:

- (5) Derivation of Schrodinger equation and the physical meanings of wave function see T. Y. Tsong, *Electronic Interpretation of Chemical Bonding*, Science Education (科學教育), Vol. 8, No. 8, (1962). Note that $\hbar = h/2\pi$.
- (6) $E = E_k + V$, where $E_k = \frac{1}{2}mv^2 = p^2/2m$.
- (7) Substitution of (1~5) into (1~1) will easily verify that it is a solution of the differential equation (1~1). Discussion of equations (1~5), (1~6) and (1~7) however will be found in elementary textbooks of physical chemistry and modern physics. A brief example is given in H. Margenau etc., *loc. cit.*, pp. 228~235.

We are considering what fraction of particles will penetrate through region II and appear in region III, if particles of kinetic energy $E_k = E$, i. e. $V = 0$, impinge on a rectangular barrier of thickness a and height V_0 . In other words, we are trying to find the probability that a particle will be reflected from or transmit through the barrier. Suppose ψ_1 , ψ_2 and ψ_3 are wave functions of the particle in regions I, II, III respectively, and let

$$\psi_1 = A e^{i\kappa_1 x} + B e^{-i\kappa_1 x} \quad (1-9)$$

$$\psi_2 = C e^{i\kappa_2 x} + D e^{-i\kappa_2 x} \quad (1-10)$$

$$\psi_3 = F e^{i\kappa_1 x} + G e^{-i\kappa_1 x} \quad (1-11)$$

where $\kappa_1 = \sqrt{2mE} / \hbar \quad (1-12)$

and $\kappa_2 = i\sqrt{2m(V_0 - E)} / \hbar \quad (1-13)$

and A, B, C, D, F, G , are coefficients to be determined. Since the first terms of wave functions stand for waves propagating from left to right, while the second terms stand for waves from right to left, the second term of ψ_3 is missing, i. e. $G = 0$, assuming that no particles hit on the barrier from region III. wave mechanics requires ψ functions to be continuous over all space, that is at contact surface

$x = 0, \psi_1 = \psi_2, \frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}^{(8)}$ and $x = a, \psi_2 = \psi_3, \frac{d\psi_2}{dx} = \frac{d\psi_3}{dx}$, From these boundary conditions

we obtain $A + B = C + D \quad (1-14)$

$$\kappa_1 (A - B) = \kappa_2 (C - D) \quad (1-15)$$

$$C e^{i\kappa_2 a} + D e^{-i\kappa_2 a} = F e^{i\kappa_1 a} \quad (1-16)$$

$$\kappa_2 (C e^{i\kappa_2 a} - D e^{-i\kappa_2 a}) = \kappa_1 F e^{i\kappa_1 a} \quad (1-17)$$

We have now four equations for five coefficients, hence we can solve the ratio for any pair of them. Our interest is in the ratio of $|F|^2 / |A|^2$. Since this value indicates the ratio of transmission, which we name transmission coefficient⁽⁹⁾ and denote it by T .

Now let us divide (1-15) by κ_1 then add it to (1-14)

$$A = \frac{1}{2} \left[\left(1 + \frac{\kappa_2}{\kappa_1}\right) C + \left(1 - \frac{\kappa_2}{\kappa_1}\right) D \right] \quad (1-18)$$

or by subtracting it from (1-14)

$$B = \frac{1}{2} \left[\left(1 - \frac{\kappa_2}{\kappa_1}\right) C + \left(1 + \frac{\kappa_2}{\kappa_1}\right) D \right] \quad (1-19)$$

Notes:

(8) $\psi_1 = \psi_2$ and $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ mean that the functions themselves and their slopes meet at $x = 0$. This implies that they are continuous at $x = 0$.

(9) Normalization and orthogonality require that $\sum_{i=1}^n \alpha_i^* \alpha_i = \sum_{i=1}^n |\alpha_i|^2 = 1$ and $\sum_{i \neq j} \alpha_i^* \alpha_j = 0$ for wave function of general form $\psi = \sum_{i=1}^n \alpha_i \psi_i$. Here α_i^* is the complex conjugate of α_i ; $|\alpha_i|^2$ represents the probability distribution of ψ to ψ_i or contribution coefficient of ψ_i to ψ . By this category, it is easy to realize that $|F|^2 / |A|^2$ is the transmission coefficient of the particles under consideration. See C. A. Coulson, *Valence*, Oxford University Press, 1952, pp. 13~19.

Again divide (1-17) by κ_2 then add it to (1-16)

$$C e^{i\kappa_2 a} = \frac{1}{2} \left(1 + \frac{\kappa_1}{\kappa_2}\right) F e^{i\kappa_1 a}$$

or
$$C = \frac{1}{2} \left(1 + \frac{\kappa_1}{\kappa_2}\right) F \exp i(\kappa_1 - \kappa_2)a \quad (1-20)$$

Substituting (1-20) into (1-16), $D e^{-i\kappa_2 a} = \frac{1}{2} \left(1 - \frac{\kappa_1}{\kappa_2}\right) F e^{i\kappa_1 a}$

or
$$D = \frac{1}{2} \left(1 - \frac{\kappa_1}{\kappa_2}\right) F \exp i(\kappa_1 + \kappa_2)a \quad (1-21)$$

Now introducing (1-20) and (1-21) into (1-18) and reducing

$$A = \frac{1}{4} F e^{i\kappa_1 a} \left[\left(2 + \frac{\kappa_1 + \kappa_2}{\kappa_2} + \frac{\kappa_2}{\kappa_1}\right) e^{-i\kappa_2 a} + \left(2 - \frac{\kappa_1 - \kappa_2}{\kappa_2} - \frac{\kappa_2}{\kappa_1}\right) e^{i\kappa_2 a} \right]$$

Rearranging $A = \frac{1}{4} F e^{i\kappa_1 a} \left[2 (e^{i\kappa_2 a} + e^{-i\kappa_2 a}) - \left(\frac{\kappa_1 + \kappa_2}{\kappa_2} + \frac{\kappa_2}{\kappa_1}\right) (e^{i\kappa_2 a} - e^{-i\kappa_2 a}) \right]$

or
$$A = F e^{i\kappa_1 a} \left[\cosh i\kappa_2 a - \frac{1}{2} \left(\frac{\kappa_1 + \kappa_2}{\kappa_2} + \frac{\kappa_2}{\kappa_1}\right) \sinh i\kappa_2 a \right] \quad (1-22)$$

Taking the complex conjugate of A ⁽¹¹⁾

$$A^* = F^* e^{-i\kappa_1 a} \left[\cosh i\kappa_2 a + \frac{1}{2} \left(\frac{\kappa_1 + \kappa_2}{\kappa_2} + \frac{\kappa_2}{\kappa_1}\right) \sinh i\kappa_2 a \right] \quad (1-23)$$

From (1-22), (1-23) we get

$$\frac{|A|^2}{|F|^2} = \frac{AA^*}{FF^*} = \cosh^2 i\kappa_2 a - \frac{1}{4} \left(\frac{\kappa_1 + \kappa_2}{\kappa_2} + \frac{\kappa_2}{\kappa_1}\right)^2 \sinh^2 i\kappa_2 a \quad (1-24)$$

If a is fairly large, $e^{-i\kappa_2 a}$ is small in comparison with $e^{i\kappa_2 a}$, therefore we may take approximation that

$$\cosh^2 i\kappa_2 a \approx \sinh^2 i\kappa_2 a \quad (12)$$

Again when $V_0 \gg E$, we see from (1-12) and (1-13) the ratio

$$\frac{\kappa_2}{\kappa_1} = i \sqrt{\frac{V_0 - E}{E}} \quad (1-25)$$

is large in magnitude, and its reciprocal κ_1/κ_2 is small that can be neglected.

Therefore (1-24) is reduced to

$$\frac{|A|^2}{|F|^2} \approx \left[1 - \frac{1}{4} \left(\frac{\kappa_2}{\kappa_1}\right)^2 \right] \sinh^2 i\kappa_2 a$$

or
$$\frac{|A|^2}{|F|^2} \approx -\frac{1}{4} \left(\frac{\kappa_2}{\kappa_1}\right)^2 \sinh^2 i\kappa_2 a \quad (1-26)$$

Notes:

(10) By definition $\sinh x = \frac{1}{2} (e^x - e^{-x})$; $\cosh x = \frac{1}{2} (e^x + e^{-x})$

(11) Note that κ_2 is imaginary, hence the first term in the bracket of equation (1-22) is real and the second term is imaginary.

(12) From Note (10), if x is large enough, e^{-x} will vanish, and $\cosh x \approx \sinh x$, that $\cosh^2 x \approx \sinh^2 x$.

(13) Since $\sinh^2 i\kappa_2 a = \frac{1}{4} [\exp (2i\kappa_2 a) + \exp (-2i\kappa_2 a) - 2]$, where κ_2 by (1-13) is equal to $i \sqrt{2m(V_0 - E) / \hbar}$, if $V_0 \gg E$, term $(2i\kappa_2 a)$ is a large negative number, hence $\exp (2i\kappa_2 a)$ approaches zero, and $\exp (-2i\kappa_2 a)$ is large in comparison with 2, therefore $\sinh^2 i\kappa_2 a \approx \frac{1}{4} \exp (-2i\kappa_2 a)$.

Introducing (1-25) into (1-26) and replacing $\sinh^2 i\kappa_2 a$ by its largest term¹³

$$\frac{|A|^2}{|F|^2} \approx \frac{1}{16} \frac{V_0 - E}{E} \exp(-2 i\kappa_2 a) \quad (1-27)$$

This is equal to

$$T = \frac{|F|^2}{|A|^2} \approx \frac{16E}{V_0 - E} \exp\left[-\frac{2}{\hbar} \sqrt{2m(V_0 - E)} a\right] \quad (1-28)$$

From this equation, we conclude that for particle of mass m so small as electrons or alpha particles, transmission coefficient T is not negligible provided that a is not too large. In fact, there is no rectangular energy barrier as shown in Figure 1. Potential energy barrier is always a smooth curve, In such a case we can practically reduce (1-28) into the form

$$T \approx \exp\left[-\frac{2}{\hbar} \int \sqrt{2m[V(r) - E]} dr\right]^{(14)} \quad (1-29)$$

II. The Band Model of Metals⁽¹⁵⁾

We recall in this section some basic ideas of band theories.

Molecular orbital theory using *LCAO*⁽¹⁶⁾ treatment states that two overlapping s orbitals, one from each of two atoms, produce two new orbitals of slightly different energies. By similar reasoning, repeated addition of one more atomic orbital produces one more molecular orbital. For j centers crystal, therefore, possesses j molecular orbitals of very close energies. These orbitals form a energy band. Between energy bands of neighboring quantum states, for instance between $1s$ and $2s$ levels, there is an energy gap. No electron is allowed to move in this gap. If the number of electrons in the crystal is such that the allowed energy bands are occupied entirely, there are no free electrons at all, and the crystal will behave as an insulator. On the other hand, if one or more bands are partly filled, the crystal will behave as a metal. Semi-conductors are crystals between two extreme examples. The partly occupied outermost band of valence electrons is a conduction band, while the next fully occupied bands of valence electrons are valence bands. And the rest of electrons in the atom form inner shell which are less important in characterizing the metallic behavior of the crystals. For three-dimensional considerations, these bands

Notes:

- (14) In (1~27), if the absolute value of exponential term is so large, term $16E/(V_0 - E)$ is no longer important, so that it can be taken as unit. Since potential energy V is a function of coordinate variable r , we can reduce (1~28) to $T \approx \exp\left[-\frac{2}{\hbar} \sum_{-1}^n \sqrt{2m[V(r_i) - E]} \Delta r_i\right] \approx \exp\left[-\frac{2}{\hbar} \int \sqrt{2m[V(r) - E]} dr\right]$.
- (15) General references are given: a). W. J. Moore, *Physical Chemistry*, 3rd ed., Prentice-Hall, Inc., 1962, pp. 680~685; b). Coulson, *loc. cit.*, pp. 276~287; c). C. Kittel, *Introduction to Solid State Physics*, 2nd ed., John Wiley & Sons, 1956, Chapt. 11; d). R. A. Smith, *Semiconductors*, Cambridge University Press, 1958, Chaps. 1, 2.
- (16) Linear Combination of Atomic Orbitals. See Coulson, *loc. cit.*, pp. 69~76.

are known as Brillouin zones.

Studies of probability distribution of conduction electron energy states in metallic crystals have been experimentally and theoretically developed by Sommerfeld, Fermi, Dirac and many other investigators. If we denote the number of energy states available per unit volume in a given crystal by N , the density of states by $g(E)$, we have

$$\int g(E) dE = NV = \frac{V}{3\pi^2 \hbar^3} (2mE)^{\frac{3}{2}} \quad (2-1)$$

$$\text{and} \quad g(E) = \frac{V}{2\pi^2 \hbar^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}} \quad (2-2)$$

where V is the volume of the crystal. The distribution curve is shown in Figure 3.

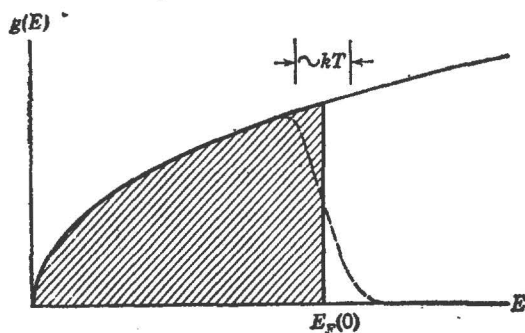


Fig. 3. Plot of density of state $g(E)$ as a function of energy. The solid line indicates the distribution at absolute zero, and the dotted line at temperature T .

III. Electrons in Metallic Crystals

Regular lattice points of metallic crystals form a set of periodic potentials. The potential energy rises rapidly to infinite at the position near each of nucleus that representing a deep potential energy well for electrons. If we plot a negative potential energy versus coordinate variable, we get a periodic potential diagram with period equal to the length of unit cell a . An oversimplified diagram for such potential barrier is shown in Figure 4. Movement of conduction electrons from the vicinity of one nucleus to that of the next requires the electrons to pass through these potential barriers. As we discussed in Section I, tunnel effect, thus plays an essential role in theorizing the energy state, and hence of metallic behavior, of electrons in metallic crystals.

Notes:

(1) Derivation of (2~1) and (2~2) see C. Kittel, *loc. cit.*, pp. 243~251.

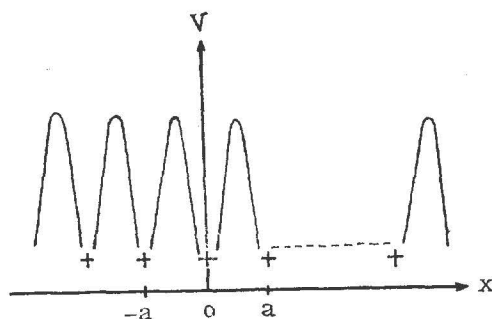


Fig. 4. Periodic negative potential energy barrier for electrons in metallic crystals.

Let us now see how wave functions of Schroedinger equation are adapted into a periodic lattice according to Bloch Theorem.⁽¹⁸⁾

One-dimensional Schroedinger equation given in (1-1) is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0 \quad (3-1)$$

Since V is periodic with period a , ψ must also be periodic. Let ψ be a linear combination of two independent real solutions $f_1(x)$ and $f_2(x)$.

$$\psi(x) = A_1 f_1(x) + A_2 f_2(x) \quad (3-2)$$

A_1 and A_2 being constants. Now if $f_1(x)$ and $f_2(x)$ are solutions of (3-1), periodicity requires that $f_1(x+a)$ and $f_2(x+a)$ must be solutions of (3-1) too.

$$\text{This implies that } f_1(x+a) = \alpha_{11} f_1(x) + \alpha_{12} f_2(x) \quad (3-3)$$

$$\text{and } f_2(x+a) = \alpha_{21} f_1(x) + \alpha_{22} f_2(x) \quad (3-4)$$

the α 's being constants. Similarly, for (3-2) we have

$$\psi(x+a) = A_1 f_1(x+a) + A_2 f_2(x+a) \quad (3-5)$$

$$\text{Hence } \psi(x+a) = (A_1 \alpha_{11} + A_2 \alpha_{21}) f_1(x) + (A_1 \alpha_{12} + A_2 \alpha_{22}) f_2(x) \quad (3-6)$$

$$\text{Let } \psi(x+a) = \lambda A_1 f_1(x) + \lambda A_2 f_2(x) \quad (3-7)$$

$$\text{This means } A_1 \alpha_{11} + A_2 \alpha_{21} = \lambda A_1 \quad (3-8)$$

$$A_1 \alpha_{12} + A_2 \alpha_{22} = \lambda A_2 \quad (3-9)$$

λ being the function to be determined. Now we have $\psi(x+a)$ in the form

$$\psi(x+a) = \lambda \psi(x) \quad (3-10)$$

For equations (3-8) and (3-9) to be satisfied, λ must be subject to the equation

$$\begin{vmatrix} \alpha_{11} - \lambda & \alpha_{21} \\ \alpha_{12} & \alpha_{22} - \lambda \end{vmatrix} = 0 \quad (3-11)$$

$$\text{or } (\alpha_{11} - \lambda)(\alpha_{22} - \lambda) - \alpha_{12} \alpha_{21} = 0 \quad (3-12)$$

This is a quadratic equation which has two roots λ_1 and λ_2 for λ . Therefore there are two corresponding solutions of the Schroedinger equation.

Notes:

- (18) See a). F. Seitz, *Modern Theory of Solids*, McGraw-Hill Book Co., 1940, Chapt. 8; b). C. Kittel, *loc. cit.*, p. 279; c). H. Margenau etc., *loc. cit.*, pp. 80~81, Floquet's Theorem.

By (3-10) $\psi_1(x+a) = \lambda_1 \psi_1(x)$ (3-13)

$\psi_2(x+a) = \lambda_2 \psi_2(x)$ (3-14)

Again, since the potential is periodic and symmetric with respect to the origin, $V(x) = V(-x)$, so that if $\psi(x)$ is a solution, $\psi(-x)$ and $\psi(x-a)$ are solutions too. Replace x by $x-a$ in (3-13)

$\psi_1(x) = \lambda_1 \psi_1(x-a)$ (3-15)

Furthermore replacing x by $-x$

$\psi_1(-x) = \lambda_1 \psi_1[-(x+a)]$

or $\psi_1[-(x+a)] = \frac{1}{\lambda_1} \psi_1(-x)$ (3-16)

Comparing equations (3-16) and (3-14) to see they are similar in form with (3-10)

Obviously $\frac{\psi_1[-(x+a)]}{\psi_1(-x)} = \frac{\psi_2(x+a)}{\psi_2(x)}$ (3-17)

This lead to the result that

$\lambda_1 \lambda_2 = 1$ (3-18)

Two sets of values for λ_1 and λ_2 are considerable.

First $\begin{cases} \lambda_1 = e^{ba} \\ \lambda_2 = e^{-ba} \end{cases}$ (3-19)

where a is the length of unit cell, b a real number. But this set is not what we wanted, since as b increases, λ_1 tends to be infinite and λ_2 vanishes.

So next we consider $\begin{cases} \lambda_1 = e^{i\mu a} \\ \lambda_2 = e^{-i\mu a} \end{cases}$ (3-20)

where μ is a real number. Both λ_1 and λ_2 in this form are wave functions of period a . And these are the functions which we look for.

Now we conclude that, since

$\psi(x+a) = \lambda \psi(x)$ (3-21)

the correct wave function in the periodic potential is the original wave function for the free electron multiplied by a wave function with the potential period a . Equation (3-21) is known as Bloch function.

The result obtained above may be expressed in more convenient way.

On putting $e^{i\mu a} = \exp i(\mu + 2n\pi/a)a$ (3-22)

Evidently, this equation holds over the whole range of the coordinate, therefore we may place x instead of a . Again if we take zero value of μ and express original wave function by $e^{i\kappa x}$, we have by (3-22)

$\psi(x+a) = \exp i(\kappa + 2n\pi/a)x = e^{i\kappa'x}$ (3-23)

This expression describes a wave travelling through the crystal in the positive x direction. For that of oppositely directed wave

$\psi[-(x+a)] = \exp -i(\kappa + 2n\pi/a)x = e^{-i\kappa'x}$ (3-24)

Notes:

(19) $e^{-i\mu a} = \cos \mu a - i \sin \mu a = \cos(\mu a + 2n\pi) - i \sin(\mu a + 2n\pi) = \exp -i(\mu a + 2n\pi) = \exp -i(\mu + 2n\pi/a)a$.

(20) From $\kappa = p/h$ and $p = h/\lambda$ we get $\kappa = \frac{2\pi}{\lambda}$.

We see from (3-23) and (3-24) that the effect of periodic potential on electrons is to modulate the frequency of original wave which is proportional to $\kappa^{(20)}$ by subjecting it to a periodic function. The general relation between κ and κ' is

$$\kappa' = \kappa \pm \frac{2n\pi}{a} \quad (3-25)$$

When $\kappa = -\kappa'$, the electron wave is completely reflected by the potential barrier, and a standing wave is set up in a unit cell. In this case

$$\kappa = \pm \frac{n\pi}{a} \quad (3-26)$$

which is an analogy to Bragg equation for reflecting wave.

$$2d \sin \theta = n\lambda \quad (3-27)$$

Since energy of an free electron is proportional to κ^2 (21), out of the boundary $\kappa = \pm \frac{n\pi}{a}$, there are no energy states allowed, and energy gaps are thus formed. On the contrary, inside the boundary, bands perfectly free for conduction electrons called, as we mentioned before, Brillouin zones are established. It is easily seen, therefore, that the electrical conductivity of metals in the idealized model, in which the nuclei are arranged at the point of perfectly periodic lattice, no resistance would be perceived. The electron wave ψ would pass through the lattice unscattered, without resistance, just like electromagnetic radiations pass through perfect medium without scattering or alteration. The resistance of metals arises only when the crystals are imperfect, for example, lattice vibration caused by heat, lattice vacancies and impurities, dislocation and many other defects of crystal lattice. These explanations are also particularly instructive to the fact that the resistivities of metals increase as the temperature rises.

金屬晶體中之洞穿效應

蘭德樂* 鄭天佑**

一、一定邊界條件下粒子對高於其總能量的位能障壁之穿透係數 T 經計算如下：

$$T \approx \frac{16E}{V_0 - E} \exp \left[-\frac{2}{\hbar} \sqrt{2m(V_0 - E)} a \right]$$

式中 E 表粒子之總能量、 m 為粒子之質量、 V_0 障壁位能、 a 障壁厚度。

二、固態晶體中價電子所成最外層能帶稱導電帶。此帶中之能位被電子所佔滿者為絕緣體；帶中留有適當空位，電子得以自由移動其間者為導體；自由電子或空位之數目甚少者為半導體。

三、金屬晶格形成週期性位能障壁。自由電子在該障壁中之波函數為其原有函數乘以另一週期為晶格軸長之波函數。

四、自由電子在理想晶體中移動所受之阻力為零。金屬之電阻係由於晶體不理想及熱振盪所致。

Note:

(2) By (1~2), $E = p^2/2m + V$, putting $V = 0$, and substituting (1~6) into it we get $E = \hbar^2 \kappa^2 / 2m$.

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