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A New Approach to Tunneling

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Abstract. A new numerical algorithm for tunneling is presented. This algorithm can be used to analyse an one-dimensional potential barrier with an arbitrary profile. It is able to calculate not only the transmission coefficient accurately, but also the phases of the transmitted and reflected waves. Using the Schrodinger equation and plane waves, we introduce a tunneling matrix to relate the transmitted and incident wave functions. Thus the transmission coefficient and phase can be calculated from the tunneling matrix. To test the accuracy of this algorithm, we calculate the transmission coefficients and phases for a double-barrier (resonant tunneling) and a triangular barrier (field emission), and make comparisons with corresponding analytical values. It shows that this algorithm is fast, accurate and efficient.

1. INTRODUCTION

The quantum tunnel effect is the theoretical foundation of various tunnel devices. Therefore the calculation of the tunneling current has been a subject of interest for many years. In order to calculate the tunneling current, the transmission coefficient must be calculated. Up to now the transmission coefficient has been calculated using various approximate methods, for example, the semi-classical method (WKB) [1-3] and the perturbation method [4]. The advantages of these methods are that they are simple in their formulae, and are able to give analytical expressions for the tunneling current in some simple cases. Their outstanding defect is that the calculated errors are large and difficult to estimate.

In this paper we present a new approach to tunneling and a corresponding algorithm for the transmission coefficient. Analysis shows that this algorithm is very accurate, and its errors can be estimated.

2. THEORETICAL PRINCIPLES

Figure 1 shows the potential profile of an one-dimensional barrier $V(x)$, where m and E are the mass and energy of incident particle, respectively. The wave function $Y(x)$ is determined from the time-independent Schrodinger equation

$$Y'' = C[V(x) - E]Y, \quad C = 2m/\hbar^2 \quad (1)$$

where the primes on $Y(x)$ indicate derivative with respect to x , and $\hbar$ is Planck's constant. On the left-hand side of the barrier there are incident and reflected plane waves,

$$Y(x) = A \exp[j(Pa + Kx)] + B \exp[j(Pb - Kx)], \quad x \leq 0 \quad (2)$$

Figure 1: One-dimensional potential barrier.

where $K = (CE)^{1/2}$, A, B and Pa, Pb are the amplitudes and phases of the incident and reflected waves (relative to the transmitted wave), respectively. On the right-hand side of the barrier there is the transmitted wave,

$$Y(x) = G(x), \quad x \geq s \quad (3)$$

where $G(x)$ is a known function determined by the boundary condition at the right-hand side of the barrier.

Under the boundary condition (3), the equation (1) can be solved by a numerical method. For example, in the Numerov algorithm [5] the difference formula corresponding to equation (1) is

$$(1 - W_i)Y_i = [(2 + 10W_{i+1})Y_{i+1} + (W_{i+2} - 1)Y_{i+2}] \quad (4)$$

$$i = N - 2, N - 3, \dots, 1, 0$$

where $Y_i = Y(x_i)$, $x_i = i\Delta x$, $s = N\Delta x$

$$W(x) = C\Delta x^2[V(x) - E]/12 \quad (5)$$

Using (3) we have

$$Y_i = G(x_i), i = N, N - 1 \quad (6)$$

Thus we can get a numerical solution of $Y(x)$ in the whole region. This algorithm has the local error $O(\Delta x^6)$, therefore its calculated results have very high accuracy.

Taking the real and the imaginary parts of the wave function, $Y(x) = Y_1(x) + jY_2(x)$, and substituting into equations (1)–(3), we get

$$Y''_\alpha = C[V(x) - E]Y_\alpha, \quad \alpha = 1, 2 \quad (7)$$

$$Y_1(x) = A\cos(Pa + Kx) + B\cos(Pb - Kx), \quad x \leq 0 \quad (8)$$

$$Y_2(x) = A\sin(Pa + Kx) + B\sin(Pb - Kx),$$

$$Y_\alpha(x) = G_\alpha(x), \quad x \geq s \quad (9)$$

On the other hand for a free particle with the wave vector K , the wave function is

$$Z(x) = \exp(jKx) = Z_1(x) + jZ_2(x), \quad -\infty < x < \infty \quad (10)$$

The corresponding equations are

$$Z''_\beta = -CEZ_\beta, \quad \beta = 1, 2 \quad (11)$$

Multiplying (7) by Z_β and (11) by Y_α , subtracting the former from the latter, and integrating from 0 to s , we get

$$[Z_\beta Y'_\alpha - Y_\alpha Z'_\beta]_0^s = KM_{\beta\alpha}, \quad \alpha, \beta = 1, 2 \quad (12)$$

where M is the tunneling matrix,

$$M_{\beta\alpha} = C/K \int_0^s Z_\beta(x) V(x) Y_\alpha(x) dx, \quad (13)$$

In these integrands the functions $V(x)$ and $Z_p(x)$ are known, and $Y_a(x)$ have numerical solutions, so these integrations can be evaluated by a numerical method, for example, the Simpson quadrature with local errors $O(\Delta x^5)$.

Substituting (8)–(10) into the left-hand side of equation (12), we get four formulae,

$$\begin{aligned} A \sin(Pa) - B \sin(Pb) &= M_{11} - G'_1(s) \cos(Ks)/K - G_1(s) \sin(Ks) \\ A \sin(Pa) + B \sin(Pb) &= M_{22} - G'_2(s) \sin(Ks)/K + G_2(s) \cos(Ks) \\ A \cos(Pa) + B \cos(Pb) &= M_{21} - G'_1(s) \sin(Ks)/K + G_1(s) \cos(Ks) \\ 4 \cos(Pa) - B \cos(Pb) &= -M_{12} + G'_2(s) \cos(Ks)/K + G_2(s) \sin(Ks) \end{aligned} \quad (14)$$

Thus A, B and Pa, Pb may be solved from (14), and the reflection and the transmission coefficients are

$$R = B^2/A^2 \quad \text{and} \quad T = 1 - R \quad (15)$$

respectively. The phases of the reflected wave and the transmitted wave (relative to the incident wave) are

$$Pr = Pb - Pa \quad \text{and} \quad Pt = -Pa \quad (16)$$

respectively.

3. APPLICATION TO DOUBLE-BARRIER

For a diode with a double-barrier tunnel junction, there is resonant tunneling. Figure 2 shows the potential profile for a rectangular double-barrier. For this case, the transmitted wave is a plane wave, $G(x) = \exp(jKx)$,

$$G_1(x) = \cos(Kx), \quad G_2(x) = \sin(Kx)$$

For this simple case, we can get an analytical formula for the transmission coefficient by solving the Schrodinger equation [9],

Figure 2: Rectangular double-barrier.

$$T_0 = 1/|Z_0|^2 \quad (17)$$

$$Z_0 = [\cosh(ql) + \frac{1}{2}ja \sinh(ql)]^2 \cdot \exp(-j2KL) + \frac{1}{4}\beta^2 \sinh^2(ql) \quad (18)$$

where $q = [C(V_0 - E)]^{1/2}$, and $\alpha = q/K - K/q$, $\beta = q/K + K/q$. The semiclassical formula (WKB) is [7]

$$T_2 = 1/|Z_2|^2 \quad (19)$$

$$Z_2 = \exp(2ql) + [\exp(2ql) - 1] \exp(j2KL) \quad (20)$$

In calculations the values of V_0, l and L are set as 0.5 eV, $5 \text{ \AA}$ and $5 \text{ \AA}$, respectively. The incident particle is an electron. Table 1 shows the calculated results, where T_1 is obtained by use of the algorithm in this paper, using $\Delta x = 0.01 \text{ \AA}$. It may be seen from the table that the values of T_1 are coincident with the values of T_0 very well. The values of T_2 have large errors.

Table 1. Transmission coefficients and phases for the rectangular double - barrier with $V_0=0.5\text{eV}$, and $l=L=5\text{\AA}$.

E(eV)	T_0	T_1	T_2	Pt	Pr
0.20	0.04068	0.04008	0.00568	-0.30833	-1.58265
0.25	0.22774	0.22604	0.01935	-0.22806	-1.09789
0.30	0.99982	0.99970	0.09261	+0.65058	-0.03770
0.35	0.46579	0.46616	0.64165	+1.33637	+1.17571
0.40	0.26352	0.26326	0.83411	+1.42434	+1.57706
0.45	0.20766	0.20727	0.63172	+1.39218	+1.83887

4. APPLICATION TO TRIANGULAR BARRIER

For the field electron emission from a metal the model potential is

$$V(x) = V_0 - eFx, \quad x > 0$$

where e and F are the magnitude of the elementary charge and the applied electric field, respectively. In order to compare with the analytical values the image force is neglected. For this case the transmitted wave is an Airy function, $G(x) = \text{Ai}(u) - j\text{Bi}(u)$, where $u = u_0 - x/\lambda$, λ is the characteristic length, $\lambda = 1/(\text{CeF})^{1/3}$ and $u_0 = C(V_0 - E)\lambda^2$.

For this simple case, we can get an analytical formula of the transmission coefficient by solving the Schrodinger equation [10],

$$T_0 = 4/(\pi K \lambda Z) \quad (21)$$

$$Z = A i^2 + B i^2 + (A i'^2 + B i'^2)/(K \lambda) + 2/\pi K \lambda \quad (22)$$

where the prime on the Airy functions Ai and Bi indicates a derivative with respect to the argument. The argument of the Airy function $\text{Ai}(u)$ and $\text{Bi}(u)$ is given by $u = u_0$. The semiclassical formula (WKB) is

$$T_2 = \exp(-4/3u_0^{3/2}) \quad (23)$$

Table 2. Transmission coefficients for the triangular barrier with $V_0=12\text{eV}$, and $F=0.5\text{V/\AA}$.

E(eV)	T_0	T_1	T_2
5	2.0344E-11	2.0345E-11	1.0275E-11
6	3.8214E-09	3.8229E-09	1.9063E-09
7	4.5839E-07	4.5855E-07	2.3261E-07
8	3.3579E-05	3.3601E-05	1.7928E-05
9	1.4005E-03	1.4015E-03	8.2620E-04
10	2.8859E-02	2.8860E-02	2.0983E-02

Figure 3. Triangular barrier.

In calculations the values of V_0 is 12eV, and the incident particle is an electron. Tables 2 and 3 show the calculated results, where T_1 is obtained by use of the algorithm in this paper, using $\Delta x = 0.01 \text{ \AA}$. In table 2 the electric field is fixed, $F = 0.5 \text{ V/\AA}$, the electron energy E is changed. In table 3 the electron energy is fixed, $E = 6 \text{ eV}$, the electric field F is changed. It may be seen from the tables that the values of T_1 are coincident with the values of T_0 very well. The values of T_2 have large errors.

Table 3. Transmission coefficients for the triangular barrier with $V_0 = 12 \text{ eV}$, and $E = 6 \text{ eV}$.

$F(\text{V/\AA})$	T_0	T_1	T_2
0.5	3.8214E-09	3.8226E-09	1.9063E-09
0.6	1.0859E-07	1.0862E-07	5.4137E-08
0.7	1.1861E-06	1.1862E-06	5.9098E-07
0.8	7.1275E-06	7.1290E-06	3.5492E-06
0.9	2.8757E-05	2.8761E-05	1.4311E-05
1.0	8.7783E-05	8.7800E-05	4.3662E-05

5. CONCLUSIONS

In this paper a new approach to tunneling is presented. The corresponding algorithm can be applied to an arbitrary one-dimensional potential barrier, and the calculated results have very high accuracy. The algorithm can calculate not only the transmission coefficient, but also the phases of the reflected and transmitted waves.

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