Quantum effects near the top of the channeling potential barrier

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2025 is the centennial of quantum mechanics.

Can quantum effects be relevant at DESY beam energies?

INTERNATIONAL YEAR OF
Quantum Science
and Technology

At $E \sim 100$ MeV there are known to exist pronounced zone structure effects in electron channeling. They are directly observable in channeling radiation. Above 200 MeV quantum effects fade out. The particle motion tends to classical, the barrier becomes impenetrable. But can tunneling effects survive for transverse energies near the barrier top even at GeV energies? Especially when the top is thin. If this is so, could it be relevant for quasichanneling? Shulga [2, 3]

Quantum effects in electron and positron channeling. II

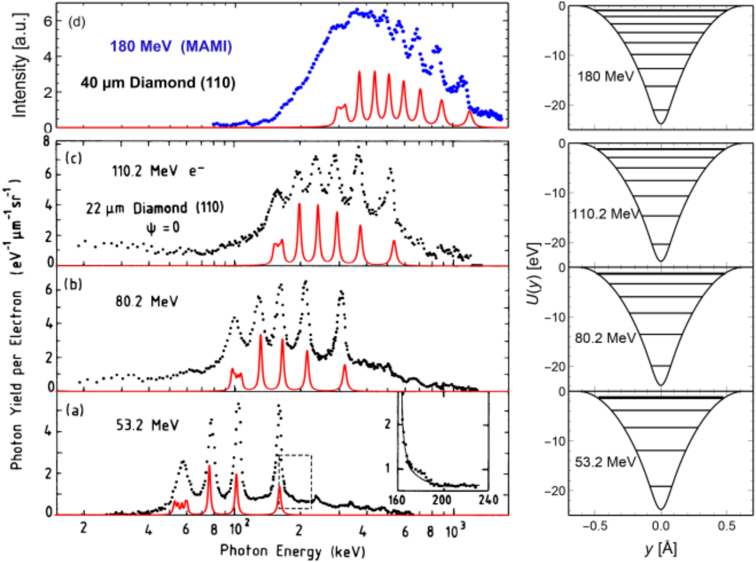

Figure 1: Photon spectra at (110) planar channeling of electrons in diamond. Spectra (a)-(c) reproduced from M. Gouanere et al. [10]. (d) deconvoluted photon spectrum taken at MAMI with a Ge(i) detector at channeling of 180

An exact representation for probability of transmission through a symmetric potential barrier. I

$$\psi''(x) + 2m\gamma\hbar^{-2}[E_\perp - V(x)]\psi(x) = 0. \tag{1}$$

$$\psi(x) \underset{x\to+\infty}{\sim} e^{\frac{i}{\hbar}\sqrt{2m\gamma E_\perp}x}. \tag{2}$$

If the crystal is not bent, the potential is symmetrical, $V(-x) = V(x)$. Then one can derive an exact representation for the transmission probability [4]

$$T(E_\perp) = \frac{1}{1 + J^{-2}\left[\frac{\partial}{\partial x}|\psi|^2\Big|_{x=+0}\right]^2}. \tag{3}$$

Here

$$\psi^*\frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^* = iJ \tag{4}$$

is imaginary and proportional to the probability current, which by virtue of Eq. (1) with $V(x)$ real is locally conserved:

$$\frac{\partial}{\partial x}J = 0, \quad \mathfrak{Im}J = 0, \quad \mathfrak{Re}J = \text{const} > 0.$$

An exact representation for probability of transmission through a symmetric potential barrier. II

Representation (3) only requires the knowledge of the wave function on one side of the potential barrier, with no need to extend it to the other side, where it converts into two oppositely running waves. The stationary scattering problem is thereby reduced from boundary to an initial-value one.

A self-suggestive approach for evaluating $\psi_+(x)$ on the $x \geq 0$ semiaxis is semiclassical approximation.

However, for application in (3) the simple WKB is unsuitable, because it breaks down in vicinity of the reflection point, which includes the point $x = 0$ if the transverse energy is close to the top of the barrier.
One should thus go beyond the simple WKB approximation.

Tunneling through a potential barrier with a round top. I

If the potential is regular near its top, it will be locally close to parabolic. In this case, the Schrödinger equation can be solved exactly, and Eq. (3) leads to the well-known result [7, 8]

$$T(E_\perp) = \frac{1}{1 + e^{2K(E_\perp)}}. \quad (5)$$

Here

$$K(E_\perp) = \hbar^{-1} \int_{x_1(E_\perp)}^{x_2(E_\perp)} dx\, u(E_\perp, x), \quad (6)$$

is the imaginary part of the classical action in units of the Planck constant $\hbar$,

$$u(E_\perp, x) = \sqrt{2m\gamma[V(x) - E_\perp]}. \quad (7)$$

The classical turning points $x_{1,2}$ (for simplicity assumed to be just two) are found from the equation

$$u(E_\perp, x_{1,2}) = 0. \quad (8)$$

Observing from (6) that $K(\max V) = 0$, from Eq. (5) one also infers that

$$T(\max V) = 1/2. \quad (9)$$

Tunneling through a potential barrier with a wedged top. I

However, the peculiarity of the mean potential of an atomic plane in channeling of positively charged particles in a crystal is that the curvature of the potential at its top is large. In the static plane approximation, the potential has a sharp point, so, the results (5), (6) do not apply.

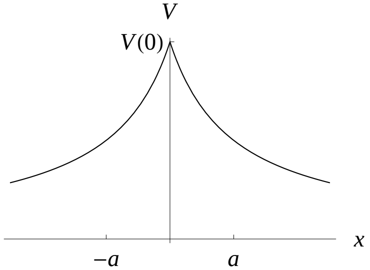

Figure 2: Schematic drawing of a static continuous potential of a single atomic plane.

Tunneling through a potential barrier with a wedged top. II

In this case, instead of WKB one can use a more accurate uniform semiclassical approximation [5, 6]

$$\psi_+(x) = \frac{1}{\sqrt{\xi'(x)}} \left\{ \mathrm{Ai}[-\xi(x)] - i\mathrm{Bi}[-\xi(x)] \right\}, \qquad x \geq 0. \tag{10}$$

Here $\mathrm{Ai}(s)$ and $\mathrm{Bi}(s)$ are the Airy functions [6], and their argument $-\xi$ is related to the x-dependent classical action:

$$\xi(E_\perp, x) = \mathrm{sgn}[E_\perp - V(x)](2m\gamma)^{1/3} \left| \frac{3}{2\hbar} \int_{x_2}^{x} \sqrt{|E_\perp - V(x)|} dx \right|^{2/3}. \tag{11}$$

Function $\xi(E_\perp, x)$ is continuous across the point $E_\perp = V(x)$.

Tunneling through a potential barrier with a wedged top. III

Note that if $E_\perp > V(0)$, $x_2(E)$ in Eqs. (6), (8) may turn out to be negative (Fig. 3b), belonging to the analytic continuation of the $x > 0$ branch of $V(x)$ potential, which physically does not exist.

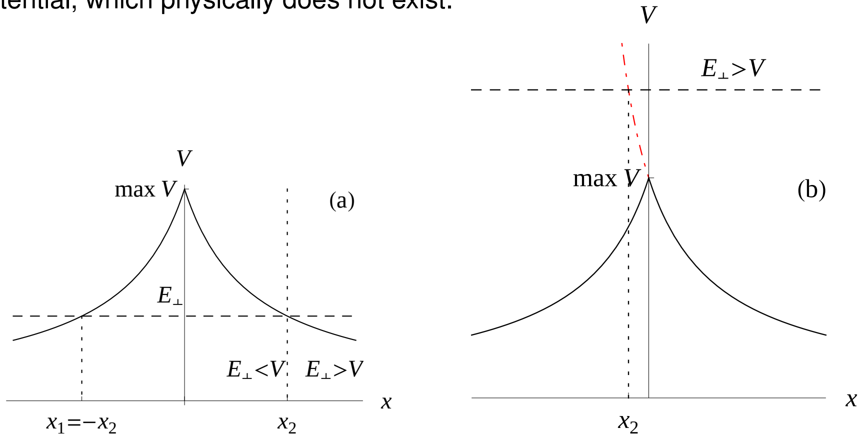

Figure 3: The real (a) and the imaginary (b) classical reflection points.

Tunneling through a potential barrier with a wedged top. IV

Employing (10), (11) in (3), one is led to the semiclassical representation for the probability of transmission through a symmetric wedge-shaped barrier:

$$T(E_\perp) = \frac{1}{1 + \frac{\pi^2}{4}\left\{(M^2)'[\xi(E_\perp, 0)] + M^2[\xi(E_\perp, 0)]\frac{\partial}{\partial x}\frac{1}{\xi'}\Big|_{x=0}\right\}^2}. \qquad (12)$$

Here

$$M^2(z) = \mathrm{Ai}^2(-z) + \mathrm{Bi}^2(-z) \qquad (13)$$

is the Airy modulus squared. It admits a single integral representation

$$M^2(z) = \frac{1}{\pi^{3/2}} \int_0^\infty \frac{dt}{\sqrt{t}} e^{-zt - t^3/12}. \qquad (14)$$

Straight-wedge approximation. I

Under semiclassical conditions, in general, $|\xi(E_\perp, 0)| \gg 1$. But ξ passes through zero at the critical transverse energy $E_\perp = \max V$. Since it grows steeply as a function of $E_\perp$, almost on the whole span of $T(E_\perp)$ it is justified to replace $\xi(E_\perp, 0)$ with its first-order Taylor expansion. This will be retrieved from (11) if one approximates the potential near its top as

$$V(x) \underset{x\to 0}{\approx} \max V - F|x|$$

with

$$F = -V'(+0) > 0, \tag{15}$$

(12) reduces to

$$T_1(E_\perp) \approx \frac{1}{1 + \left\{\frac{\pi}{2}(M^2)'\left[\Xi(E_\perp)\right]\right\}^2} \tag{16}$$

with

$$\Xi(E_\perp) = \frac{E_\perp - \max V}{\Omega}, \tag{17}$$

$$\Omega(F) = (\hbar F)^{2/3}(2m\gamma)^{-1/3}. \tag{18}$$

Straight-wedge approximation. II

The transverse energy scale parameter Ω is proportional to $\hbar^{2/3}$, in this sense being semiclassically small. However, let us estimate it for a real crystal – e.g., silicon in orientation (110). In this case $F \sim 60$ eV/Å, yielding

$$\Omega \approx \begin{cases} 24\gamma^{-1/3}\ \text{eV} & \text{for positrons} \\ 2\ \text{eV} & \text{for nonrelativistic protons or GeV positrons.} \end{cases} \quad (19)$$

This is to be compared with the potential well depth ~ 20 eV.
After simplification of the function M^2, $T(E_\perp)$ can be rendered basically the same structure as (5) for the parabolic potential barrier:

$$T(E_\perp) \approx \frac{1}{1 + e^{2\tilde{K}(E_\perp)}}, \quad (20)$$

with

$$\tilde{K}(E_\perp) = -2C_1\Xi - \frac{1}{2}\ln 3. \quad (21)$$

Herein, however, the centre of (20) is shifted to the value

$$E_\perp \approx \max V - C\Omega, \qquad C = \frac{\ln 3}{4C_1} \approx 0.377, \quad (22)$$

as is illustrated by Fig. 4.

Straight-wedge approximation. III

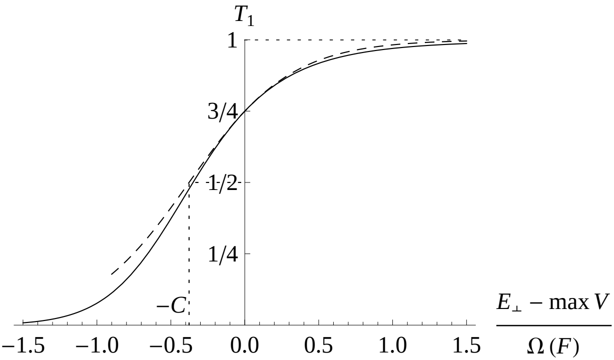

Figure 4: Solid curve, the transmission probability in the straight wedge approximation for the potential barrier, Eq. (16) with M^2 evaluated by (14). Dashed, the approximation (20), (21).

Curved-tip approximation. I

The accuracy of the approximation (16), (17) can be improved by going one step beyond the rectilinear angle approximation for the barrier, and expanding the potential near its top to the second order in x:

$$V(x) \underset{x\to+0}{\simeq} \max V - Fx + \frac{1}{2}V''(+0)x^2. \tag{23}$$

The effect of the correction is to steepen the crossover – see Fig. 5.
In particular, at the critical energy $E = \max V$, the transmission probability equals $3/4$ plus a potential curvature correction, which is positive for $V''(0) > 0$, in spite that the curved potential barrier is broader than its straight-wedge approximation:

$$T_2(\rho, \max V) \underset{\rho\ll 1}{\simeq} \frac{3}{4}\left(1 + \frac{\rho}{10C_1}\right). \tag{24}$$

with

$$C_1 = \frac{12^{1/3}\sqrt{\pi}}{\Gamma(1/6)} = 0.73, \tag{25}$$

$$\rho = \frac{V''(+0)\Omega}{F^2}. \tag{26}$$

Curved-tip approximation. II

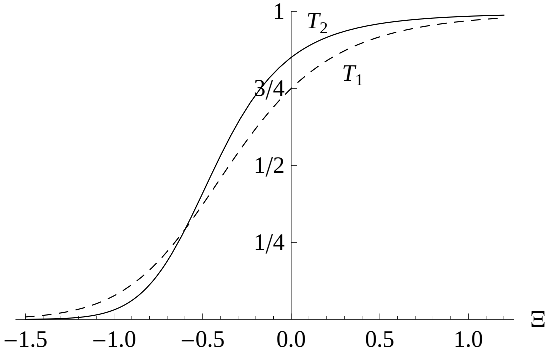

Figure 5: Solid curve, $T_2(\rho, \Xi)$ for $\rho = 1$. Dashed, the approximation (20), (21).

Conclusions

The wedged shape of the potential barrier for positively charged channeled particles increases the barrier transmissivity due to quantum effects. The sizable value of Ω for GeV positrons indicates that quantum effects in their planar quasichanneling can be discernible.

But how do these effects manifest themselves?

They can be visible at transverse energies respective to the top $E_{\perp} - \max V \sim \Omega \sim 2$ eV, which correspond to quasichanneling. In this regime, there are various effects, such as rechanneling and volume capture, for which there is tension between theory and experiment in the GeV energy range. In this case, quantum effects may be worth taking into account.

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