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The relative error of calculations at the Pöschl-Teller model potential for the planar channeled muon

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Abstract: In the framework of quantum mechanics, we investigate muon channeling in the Si (200) crystal. The transverse energy levels and wave functions are obtained for the Pöschl-Teller and the Doyle-Turner potentials. Comparative analysis demonstrates that analytical results of calculations obtained on the base of the Pöschl-Teller potential are in a good agreement with the numerical results of calculations in the Doyle-Turner model for the low energy levels. These results for the muon with rest mass m_μ and relativistic factor γ are valid for any particle with elementary charge and rest mass m and relativistic factor $\gamma_m = \gamma(m_\mu/m)$. Therefore, our results can be useful for the preparation and performing the experimental investigation of the various phenomena accompanying particle channeling.

Keywords: Interaction of radiation with matter; X-ray generators and sources

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Contents

1 Averaged channeling potentials

It is well known that when the fast charged particle penetrates into an aligned crystal, we deal with coherent scattering [1] (an ultrathin crystal) and channeling effect (thick enough crystal), which can be presented as a classical or quantum motion of particles in the electric field of periodic continuous (average) potential of crystallographic planes or axis [2].

In the well known paper [3], it was shown that relativistic charged particle will be captured in the channeling state when it enters into the crystal at a small angle (not more than some critical one — θ_L) with respect to the crystal planes or axis.

Further we shall consider only planar channeling. Obviously, the potential of the system of crystal planes is the sum of the potentials of the individual planes (taking into account the symmetry of the crystal). Due to the periodicity of the crystal structure, this potential will be periodic too.

As it was noted in the book [4] H. Bethe was the first who understand importance of consideration of "systematic" reflection for correct description of potential. In this book the connection of crystal potential with structure scattering amplitudes was discussed in detail. Doyle and Turner [5] proposed using the form factor of the crystal atoms to obtain any continuous potential with accuracy which is very close to the "real" potential. In the work [6] using the same approach the potential for proton channelling in Si crystal was obtained and used in experiments. Unfortunately, there is a problem all calculation should be done by numerical methods.

In order to obtain analytical solution it is necessary to use model potentials. One of the simplest and most accurate models is the modified Pöschl-Teller potential. The analytical solutions can be obtained only for potential of an individual plane, and unluckily, those solutions did not allow correctly describe the band structure of the energy levels of the transverse motion. Therefore, it is very important to compare the results obtained by the numerical calculation and analytical results. Such comparison of the results obtained within the framework of the Doyle-Turner model and Pöschl-Teller, still was not carried out.

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The purpose of our work is to compare the results of calculations within the framework of the quantum theory of the energy spectrum and matrix elements for planar channeled charged particles using two models of the averaged potential: Doyle-Turner(DT) and the Pöschl-Teller(PT).

Since the results obtained for muons μ^- with relativistic mass γm_μ are also valid for any particles with rest mass m, elelementary charge and relativistic factor $\gamma_m = \gamma(m_\mu/m)$, we restrict our consideration to muons. From the other hand, the muon channeling still was not investigated in detail both theoretically and experimentally.

As any relativistic fermions the muon in an external field is described by the Dirac equation. In the well-known papers [7–9] it was shown that longitudinal motion of a relativistic channeled particle can be described by plane wave, and the Dirac equation describing the transverse motion is simplified to the Schrödinger-like equation, i.e. with relativistic mass

$$\hat{H}\phi_n(x) = \left(\frac{\hat{p}^{\,2}}{2m_\mu\gamma} + U(x)\right)\phi_n(x) = E_n\phi_n(x)\,, \tag{1.1}$$

where $m_\mu\gamma$ is the muon relativistic mass, γ is the relativistic factor, $\phi_n(x)$ is the muon wave function, n denotes numbers of the particle quantum states.

Energy levels and wave functions of the relativistic muon in the crystal field $U(x)$ can be obtained by solving this Schrödinger-like equation (1.1).

1.1 The modified Pöschl-Teller potential

The modified PT potential is

$$U(x) = -\frac{U_0}{\cosh^2\alpha x} \tag{1.2}$$

here α is the parameter defining the width of the PT potential well and U_0 is the depth of this potential well. For this potential it is known several different analytical solutions of the Schrödinger equation (see, refs. [10–12]). For our task, it is convenient to use the solution obtained in [12]:

$$E_n = -\frac{U_0}{q(q+1)}(q-n)^2\,,\quad q(q+1) = \frac{2m_\mu U_0}{\hbar^2\alpha^2}\,. \tag{1.3}$$

Here E_n is the transverse energy and the wave functions are

$$\psi_n^q(x) = (\cosh(\alpha x))^{n-q}C_n^{q-n+\frac{1}{2}}(\tanh(\alpha x))\,, \tag{1.4}$$

where C_n^q are the Gegenbauer polynomials. In ref. [13] the modified PT potential was used to calculate the resonances at small-angle reflection of X-ray radiation from relativistic electrons.

According to quantum mechanics the energy level number N_E should be integer one, therefore, from eq. (1.3) for energies E_n in the PT potential it follows that

$$N_E = IntegerPart\left[\frac{1}{2}\left(\sqrt{\frac{8\gamma U_0 m}{\alpha^2\hbar^2}+1}-1\right)\right]\,. \tag{1.5}$$

In order to obtain the reliable results of calculations using the modified PT potential, one have to define the parameters U_0 and α of the potential (1.2) so that the periodic potential built from the PT potentials would be close to the periodic potential of the DT model. Our calculations for Si(220) crystal give $U_0 = 21.5$ eV, $\alpha = 3.5$ 1/Å.

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1.2 The Doyle-Turner potential

For the DT potential of the crystal planes system due to their periodic arrangement the wave functions should be the Bloch one [14]

$$\psi_n(x) = e^{i\,k_x x} \sum_m C_n(g_m, k_x) e^{-i\,g_m x}\,, \tag{1.6}$$

here $g_m = mg$, $g = |\boldsymbol{g}|$, $\boldsymbol{g}$ is the reciprocal lattice vector in the first Brillouin zone of the system of channeling planes and m is the natural number.

According to Bloch theorem [14] the Fourier components $C_n(g_m, k_x)$ of the channeled particle wave functions $\psi_n(x)$ in the momentum space should satisfy the algebraic system of equations for the eigenvalues:

$$\sum_m A_{ml} C_n(g_m, k_x) = E_n(k_x) C_n(g_m, k_x)\,, \tag{1.7}$$

Here matrix A_{ml} is (see, [15, 16])

$$A_{ml} = U(g_m - g_l) + \delta(g_m, g_l) \left[\frac{\hbar^2 (g_l + k_x)^2}{2 m_\mu \gamma} \right]\,, \tag{1.8}$$

and values $U(g_m)$ are the Fourier components of the DT periodic potential $U(x)$.

We should note that unlike the PT model, the possible energy values $E_n(k_x)$ of the channeled particle in the DT periodic potential $U(x)$ are continuous functions of the wave vector of the particle k_x, i.e. form energy bands.

The numerical solution of the system (1.7) for the DT potential gives the energy spectrum (i.e., the values $E_n(k_x)$) and the Fourier components $C_n(g_m, k_x)$ of the wave function of the channeled particle. We used the package of symbolic-numerical computations Mathematica© from our previous works [17].

The figure 1 shows the calculation of the energy levels' number of the transverse motion (bands for the DT potential) for the relativistic muon channeled in Si(220).

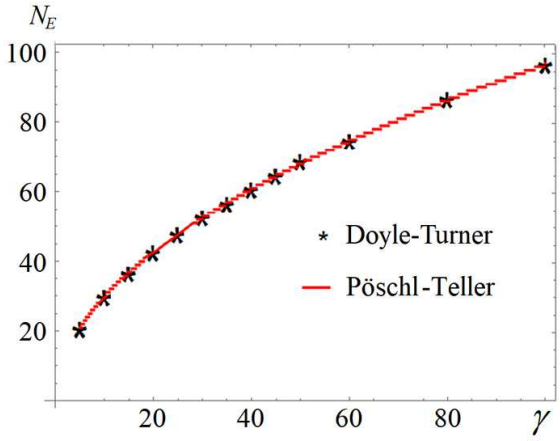

Figure 1. Dependence of the number N_E of the energy levels (bands) of the muon transverse motion in Si(220) on the μ relativistic factor γ: stars — for the Doyle-Turner potential and stepped line — for the periodic potential on the basis of the Pöschl-Teller model potential.

One can see that the results of calculations are in good agreement.

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2 Muon planar channeling

2.1 The relative error of energy spectrum

For the reason discussed above, the calculation of the energy levels' number in the transverse motion of the relativistic channeled muon can be carried out with equal accuracy using both the PT and the DT models.

To estimate the calculation error of the transverse energies of muon in the PT potential (in comparison with the values obtained in the DT model), we introduce the quantity

$$\Delta E_n = \frac{E_n - E_n(k_x)}{E_n}\,, \tag{2.1}$$

where E_n is the transverse energy of the muon channeled in Si(220) (eq. (1.3)) according to PT model and $E_n(k_x)$ is calculated by the DT model (eqs. (1.7)–(1.8)).

The figure 2 shows the results of calculations of the relative error ΔE for a muon channeled in Si(220) (taking into account the band structure $E_n(k_x)$).

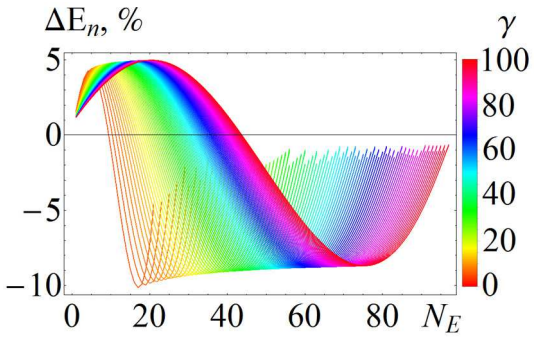

Figure 2. The dependence of the relative error ΔE_n as a function of the N_E level number and the relativistic factor γ.

The figure 2 shows that for all relativistic factors the relative error ΔE_n changes with increasing of the number N_E(transverse energy) as it follows:

- for the ground state value ΔE_n is order of 1%;
- after that value ΔE_n increases up to 5% for bound energy approximately equal to one quarter of the potential well;
- on the next step the value ΔE_n decreases to zero when muon energy achieves the middle of the potential well;
- after that the value ΔE_n again increases up to 10% for bound energy approximately equal to three quarter of the potential well;
- and finally the value ΔE_n decreases to zero for muon energy near to the top of the potential well.

2.2 The relative error of matrix elements

The wave functions and energy levels obtained above allow to estimate the error of the calculations based on the model potential of PT for many physical processes.

For example, in order to calculate the probability of different types of radiation from relativistic channeled particles, we need two parameters: the energy of the photon $\hbar\Omega_{if} = E_i - E_f$, arising during the spontaneous transition $i \to f$ between the quantum states of transverse motion and matrix elements $x_{if} = \langle\psi_f(x)|xe^{-ik_x x}|\psi_i(x)\rangle$ corresponding to this transition.

To estimate the calculation errors of the photon energy and matrix elements in the PT potential we introduce the quantities

$$\Delta\Omega_{if} = \frac{\Omega_{if}^{PT} - \Omega_{if}^{DT}}{\Omega_{if}^{DT}}, \quad \Delta X_{if} = \frac{(x_{if}^2)^{PT} - (x_{if}^2)^{DT}}{(x_{if}^2)^{DT}}, \tag{2.2}$$

where the index PT indicates the calculation results according to the Pöschl-Teller model and the DT index indicates the calculation results according to the Doyle-Turner model.

The figure 3 shows the calculation results of the relative errors $\Delta\Omega_{if}$ and ΔX_{if} for transitions between adjacent levels of muon channeled in Si(220)(i.e. $\Delta\Omega_{i,i-1}$ and $\Delta X_{i,i-1}$).

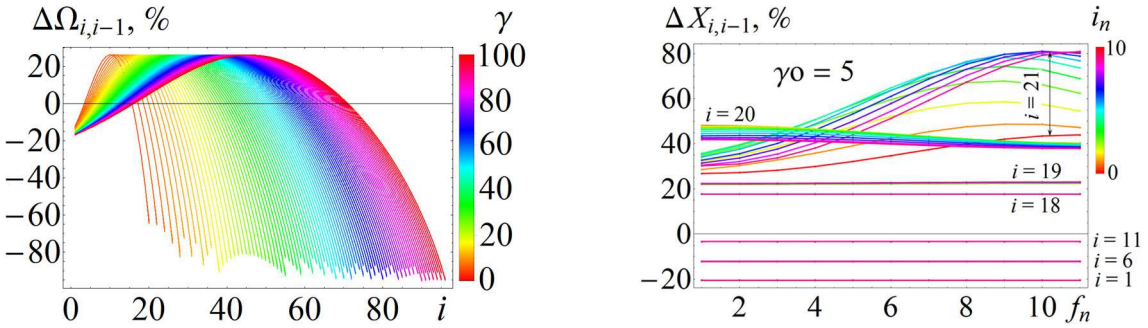

Figure 3. It is shown relative errors $\Delta\Omega_{i,i-1}$ and $\Delta X_{i,i-1}$ for transitions between neighbor levels for muon channeled in (220) Si. In the left figure the relative error of photon energy $\Delta\Omega_{i,i-1}$ is plotted as a function of the initial level number i and the relativistic factor γ. In the right picture the relative error of matrix elements $\Delta X_{i,i-1}$ is shown versus the initial level number at the $\gamma = 5$. Here, i_n and f_n are the number of the subband (we divided each band into 10 parts).

In order to take into account the width of energy band during calculation of matrix elements (in DT model), we divide every energy band into 10 subbands and consider all possible transitions.

3 Conclusion

We compare the calculation results of the number N_E of the bound states, the energy spectrum E_n, photon energies $\Delta\Omega_{i,i-1}$ and the matrix elements $\Delta X_{i,i-1}$ for muon channeled in Si(220) for two Pöschl-Teller and Doyle-Turner potentials. The main results are as follows:

- the number N_E of the muon bound states is in good agreement;
- the relative error of transverse muon energy does not exceed 10%;

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- the relative errors of photon energies and the matrix elements is in a good agreement only for the muon energy levels far from the top of the potential well. Such a behavior of these quantities is connected with the fact that when transverse energy of muon approaching to the top of the potential well, the energy bands expand and the band structure plays an increasing role. Consequently, one can use the Pöschl-Teller potential **only** in order to obtain the estimation of the phenomena connected with the low energy levels of channeled particle's transverse motion.

Our results for the muon with rest mass m_μ and relativistic factor γ are valid for any particles with elementary charge and rest mass m and relativistic factor $\gamma_m = \gamma(m_\mu/m)$. Therefore, one can be useful in the preparation and carrying out the experimental investigation of the various phenomena accompanying particle channeling.

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