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Quantum Dynamics of Positrons in the Channeling in Carbon Nanotubes

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The positrons quantum channeling in carbon nanotubes by the numerical solution of the Schrödinger equation in the corresponding paraxial approximation is considered. The spatial redistribution of the positrons flux in the transverse plane during channeling in nanotubes is detected. Also the angular distribution of positrons passed through the nanotube is studied. This distribution is sensitive to the transverse structure of nanotubes or CNT bundles. The continuum interaction potential of the positron and nanotube is obtained as a sum of continuous potentials of individual atomic chains [1]. In general, such a potential for of CNTs does not have azimuthal symmetry. For the potential of the interaction between the positron and the carbon atom we use Doyle-Turner approximation.
There are various methods for integration of time-dependent Schrodinger equation [2-4]. For the numerical integration of the Schrödinger equation we have considered the evolution operator splitting method based on the Trotter formula [5]. The initial positron beam is represented as a wide Gaussian wave packet in tranverse plane.The calculations on the grid are performed by the transition to the momentum representation using fast discrete Fourier transform algorithms. The wave function evolution was considered on a square computation domain on the transverse plane, large enough so that the interaction of the wave packet with the nanotube walls was going far away from the boundaries of the computation domain. In order to avoid the non-physical wave packet reflections at the grid boundaries an imaginary absorbing potential is introduced.

References

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