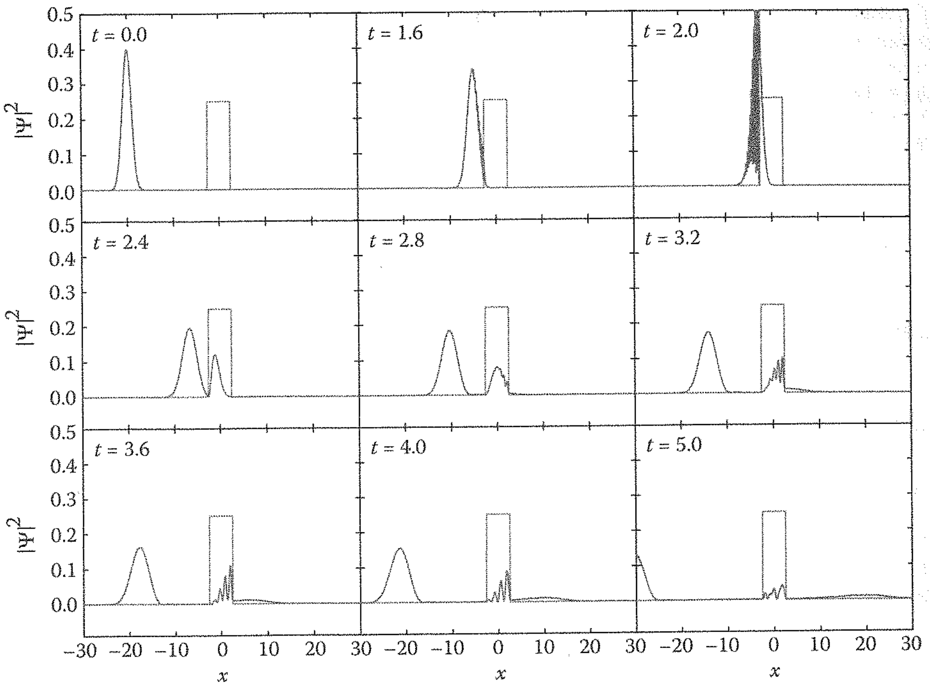

FIGURE 13.12 Scattering of a Gaussian wave packet on a square potential barrier, calculated with Program 13.14, using the tridiagonal technique for complex systems implemented in routine PropagQTD. The average energy is equal to the barrier height ($k_0^2/2 = V_0 = 50$).

For reasons of consistency with the overall philosophy of using real arithmetic, Program 13.15 defines a distinct routine InitR for initializing the real and imaginary components of the wave packet, and a routine ProbDensR for evaluating the normalized probability density. The rest of the functionalities are identical with those of Program 13.14. Snapshots from an actual run are depicted in Figure 13.13. One can readily notice that reflected waves are produced even though the reflection probability of a classical particle under the same conditions is zero.

Even though the strategy using Gauss–Seidel iterations and real arithmetic for solving the discretized Schrödinger equation (implemented in routine PropagQGS) is somewhat slower than the dedicated LU factorization technique for complex linear systems (implemented in routine PropagQTD), the former is more amenable in situations of higher complexity, as, for instance, higher dimensionality or more sophisticated boundary conditions.

Listing 13.15 Scattering of a Quantum Wave Packet Using a Gauss–Seidel Solver (Python Coding)

```
# Reflexion/transmission of quantum wave packet using Gauss-Seidel solver
from math import *
from pde import *

def Pot(x, a, V0):                                               # Potential
   return V0 if fabs(x) <= 0.5e0*a else 0e0

#============================================================================
def InitR(Psi, Chi, x, nx, x0, sig, k0):
#----------------------------------------------------------------------------
#  Initial Gaussian wave packet
```