

Erratum: Boundary conditions for the Schrödinger equation in the numerical simulation of quantum systems [Phys. Rev. E **50**, 1616 (1994)]

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In the Appendix of this paper there is an error in the expressions of coefficients β_j , and r_j of the finite-difference Schrödinger equation used in the numerical simulations, $\alpha \psi_{j+1}^{k+1} + \beta_j \psi_j^{k+1} + \alpha \psi_{j-1}^{k+1} = r_j$, where ψ_j^k is the wave function $\psi(x, t)$ at position $x = x_j$ and time $t = t_k$.

The correct Eqs. (A4)–(A7) defining the coefficients are

$$\alpha = -i\Delta t/2\Delta x^2, \quad (\text{A4})$$

$$\beta_j = 1 + i\Delta t/\Delta x^2 + i\Delta t(V_j^{k+1} + V_j^k)/2, \quad (\text{A5})$$

$$r_j = \alpha^* \psi_{j+1}^k + \bar{\beta}_j \psi_j^k + \alpha^* \psi_{j-1}^k, \quad (\text{A6})$$

where

$$\bar{\beta}_j = 1 - i\Delta t/\Delta x^2 - i\Delta t(V_j^{k+1} + V_j^k)/2, \quad (\text{A7})$$

where the terms V_j^k and V_j^{k+1} (potential at position $x = x_j$ and times $t = t_k$ and $t = t_{k+1}$, respectively) now have opposite signs. Furthermore, if absorbing boundary conditions are used, the external (real) potential $V(x, t)$ has to be replaced with the total (complex) potential $(V + iV_i)$, where $iV_i(x)$ is the absorbing (imaginary) potential.