

Erratum: Numerical simulation of mesoscopic systems with open boundaries using the multidimensional time-dependent Schrödinger equation [J. Appl. Phys. 69, 7153 (1991)]

Leonard F. Register, Umberto Ravaioli, and Karl Hess
*Beckman Institute and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign,
 Urbana, Illinois 61801*

The article contains a few notational and typographical errors that should be corrected as follows: In Sec. II A, the continuum effective mass Hamiltonian should be $H = -(\hbar^2/2m^*)\nabla^2 + V(r)$. In Sec. II B, Eq. (7) should read

$$\begin{aligned} \psi_{\text{left}}(x) &\simeq ae^{ikx} + (b_l + c_px)e^{-ikx} \\ \psi_{\text{right}}(x) &\simeq (b_r + c_r x)e^{ik'x}. \end{aligned} \tag{7}$$

Again, in Sec. II B, the last paragraph should begin:

For the example calculations presented in the next section, we chose the following simple scheme, in the form of Eq. (8):

$$\langle \mathbf{R}_b + \hat{\mu}\Delta | \psi(t) \rangle \simeq \left[\prod_{l=0}^L \langle \mathbf{R}_b - \hat{\mu}l\Delta | \psi(t_n) \rangle^{a_l} \right] \left[\sum_{l=0}^L a_l \frac{\langle \mathbf{R}_b - \hat{\mu}l\Delta | \psi(t) \rangle}{\langle \mathbf{R}_b - \hat{\mu}l\Delta | \psi(t_n) \rangle} \right], \tag{10}$$

where \mathbf{R}_b is a boundary site and $\hat{\mu}$ is a unit vector normal to the boundary and directed outwards, as shown in Fig. 1. An appropriate choice of the coefficients a_l provides any desired polynomial curve fit near the boundary. For example, for a linear curve fit, $a_0=2, a_1=-1, a_{l>2}=0$ and for a parabolic curve fit, $a_0=3, a_1=-3, a_l=-3, a_2=1, a_{l>3}=0$.

Finally, in Sec. III B, contrary to the text but in agreement with the caption of Fig. 3, the stub length was switched from 70 to 110 Å.