

Corrections

The multiconfiguration time-dependent Hartree (MCTDH) method: A highly efficient algorithm for propagating wavepackets

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In Eqs. (B.31), (B.33), and (B.40) a "π" is missing.

In Eq. (B.43) the expression $(l+m)!/(l-m)!$ is to be replaced by its reciprocal value.

In Eq.(B.51) c_{l-1}^2 must be replaced by c_{l+1}^2

In Eq.(B.65) $-\frac{1}{3}$ must be replaced by $\frac{1}{3}$

The corrected equations read:

$$\begin{aligned} \varphi_j(x) &= (2^j j!)^{-1/2} (m\omega/\pi)^{1/4} H_j(\sqrt{m\omega}(x-x_{\text{eq}})) \\ &\quad \times \exp\left(-\frac{1}{2} m\omega (x-x_{\text{eq}})^2\right) \end{aligned} \quad (\text{B.31})$$

$$w_\alpha^{1/2} = (m\omega/\pi)^{-1/4} \exp\left(\frac{1}{2} m\omega (x_\alpha - x_{\text{eq}})^2\right) U_{0\alpha} \quad (\text{B.33})$$

$$w_\alpha^{1/2} = \pi^{1/4} (m\omega)^{-3/4} (x-x_0)^{-1} \exp\left(\frac{1}{2} m\omega (x_\alpha - x_{\text{eq}})^2\right) U_{1\alpha} \quad (\text{B.40})$$

$$\varphi_{l-m+1}(\theta) = \tilde{P}_l^m(\theta) = (-1)^m \sqrt{\frac{2l+1}{2} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) \quad (\text{B.43})$$

$$c_{l+2} c_{l+1} \tilde{P}_{l+2}^m(x) + (c_l^2 + c_{l+1}^2 - x^2) \tilde{P}_l^m(x) + c_l c_{l-1} \tilde{P}_{l-2}^m(x) = 0 \quad (\text{B.51})$$

$$D_{\alpha\beta}^{(2),\text{DVR}} = -\left(\frac{\pi}{\Delta x}\right)^2 \begin{cases} \frac{1}{3} + \frac{1}{6(N+1)^2} - \frac{1}{2(N+1)^2 \sin^2\left(\frac{\alpha\pi}{N+1}\right)}, & \alpha = \beta \\ \frac{2(-1)^{\alpha-\beta}}{(N+1)^2} \frac{\sin\left(\frac{\alpha\pi}{N+1}\right) \sin\left(\frac{\beta\pi}{N+1}\right)}{\left(\cos\left(\frac{\alpha\pi}{N+1}\right) - \cos\left(\frac{\beta\pi}{N+1}\right)\right)^2}, & \alpha \neq \beta \end{cases} \quad (\text{B.65})$$

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