One-dimensional model potentials for strong-field simulations

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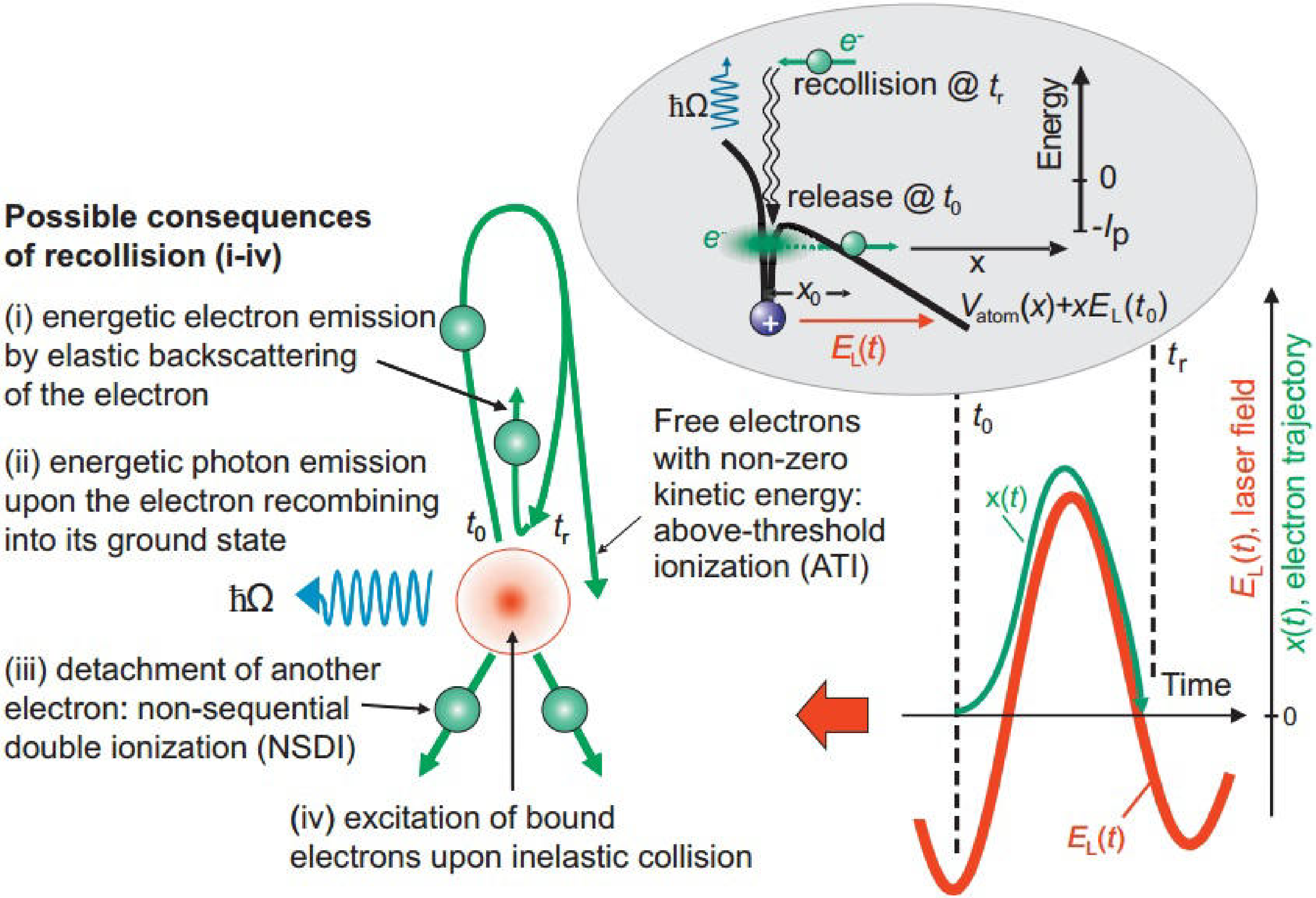
Outline

- Motivation
- Construction of the density-based 1D model potential
- Improved 1D model potentials
- Simulation results
- Conclusions

Motivation

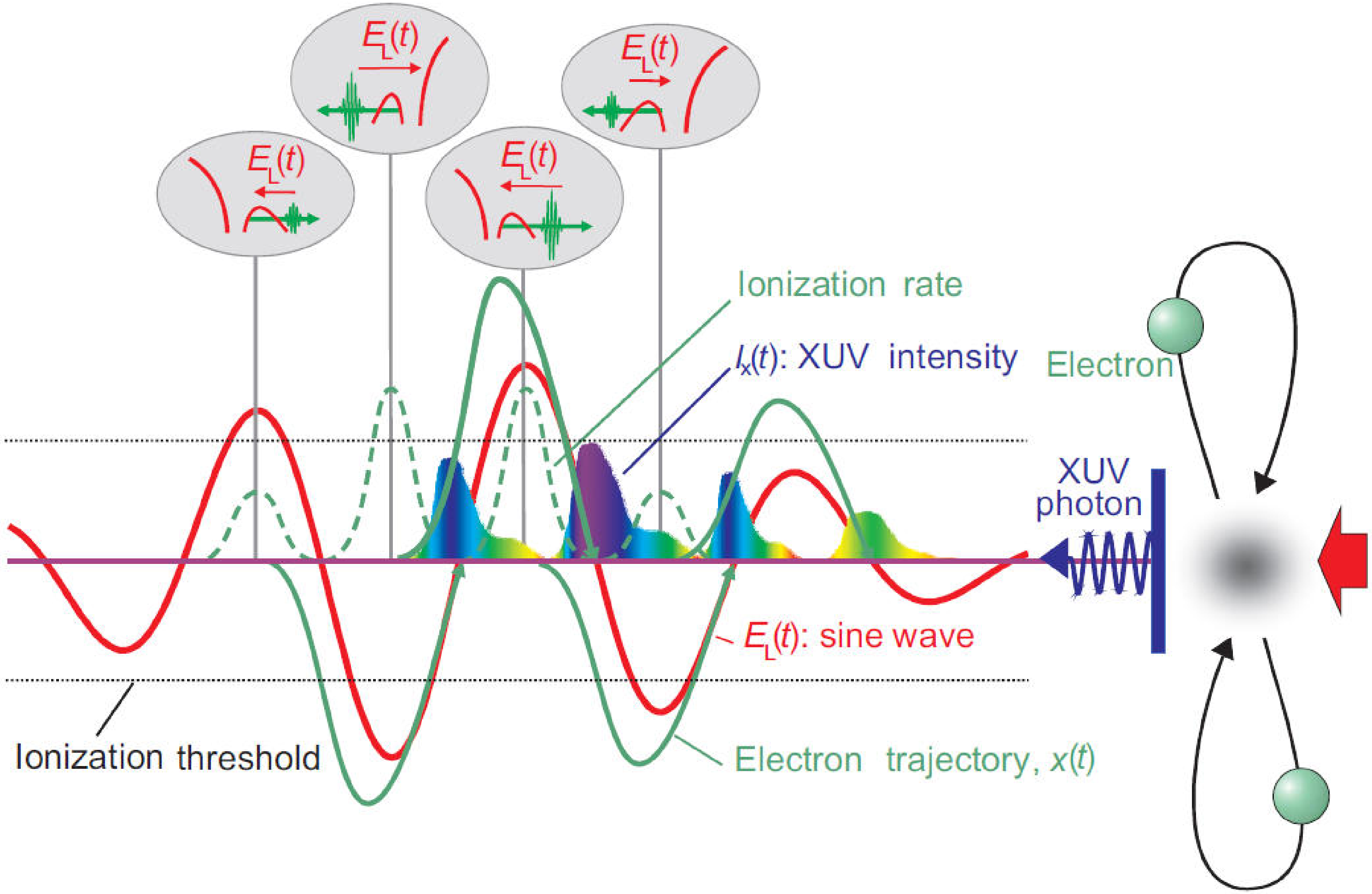
- The true understanding of the phenomena in attosecond and strong-field physics often needs the quantum evolution of an involved atomic system driven by a strong laser pulse
- Exact solution of the corresponding Schrödinger equation is beyond reach in this non-perturbative range, except for the simplest cases. Therefore, approximations are unavoidable and very important.
- For linearly polarized pulses, the main dynamics happens along the electric field of the laser pulse which underlies the success of some 1D approximations.

Motivation



[1] F. Krausz and M. Ivanov. Attosecond physics. Reviews of Modern Physics, 81, 2009.

Motivation



[1] F. Krausz and M. Ivanov. Attosecond physics. Reviews of Modern Physics, 81, 2009.

Construction of the density-based 1D model potential

- A general 3D simulation:

$$H_0^{\mathrm{3D}} = T_z + T_\rho - \frac{Z}{\sqrt{\rho^2 + z^2}}$$

$$T_\rho = -\frac{1}{2\mu}\left[\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho}\right] \qquad T_z = -\frac{1}{2\mu}\frac{\partial^2}{\partial z^2}$$

$$H_0^{\mathrm{3D}}\psi_{100}(z,\rho) = E_0\psi_{100}(z,\rho)$$

$$E_0 = -\frac{\mu Z^2}{2}, \qquad \psi_{100}(z,\rho) = \mathcal{N}\, e^{-\mu Z\sqrt{\rho^2+z^2}}$$

Construction of the density-based 1D model potential

- A general 3D simulation:

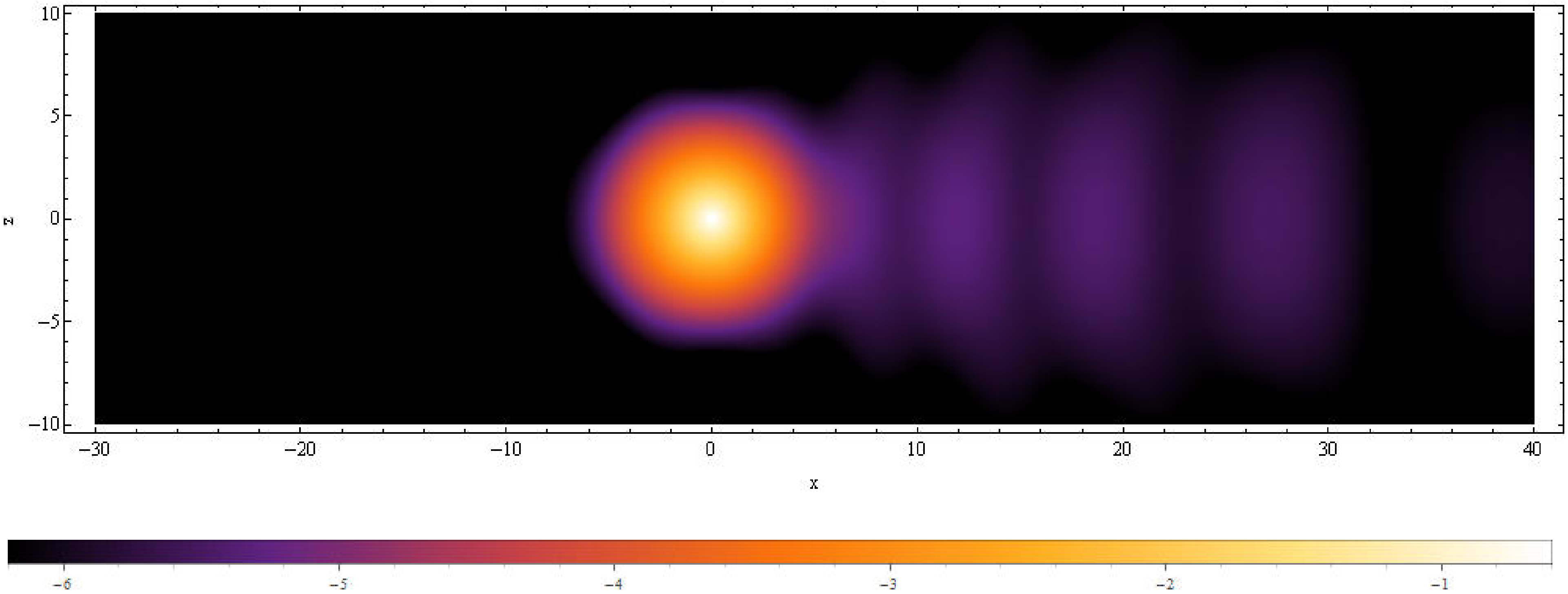
$$V_{\text{ext}}(z,t) = z \cdot \mathcal{E}_z(t)$$

$$i\frac{\partial}{\partial t}\Psi^{3\text{D}}(z,\rho,t) = \left[H_0^{3\text{D}} + V_{\text{ext}}(z,t)\right]\Psi^{3\text{D}}(z,\rho,t)$$

Initial state:

$$\Psi^{3\text{D}}(z,\rho,0) = \psi_{100}(z,\rho) = \mathcal{N}\, e^{-\mu Z\sqrt{\rho^2+z^2}}$$

3D H-atom optical tunneling



Sz. Majorosi and A. Czirják, Comp. Phys. Comm. **208**, 9-28, (2016)

Construction of the density-based 1D model potential

- A general 1D simulation:

$$i\frac{\partial}{\partial t}\Psi^{1\mathrm{D}}(z,t) = \left[H_0^{1\mathrm{D}} + V_{\mathrm{ext}}(z,t)\right]\Psi^{1\mathrm{D}}(z,t)$$

$$H_0^{1\mathrm{D}} = T_z + V_0^{1\mathrm{D}}(z) \qquad V_{\mathrm{ext}}(z,t) = z\cdot\mathcal{E}_z(t)$$

Construction of the density-based 1D model potential

- A general 1D simulation:

$$i\frac{\partial}{\partial t}\Psi^{1\mathrm{D}}(z,t) = \left[H_0^{1\mathrm{D}} + V_{\mathrm{ext}}(z,t)\right]\Psi^{1\mathrm{D}}(z,t)$$

$$H_0^{1\mathrm{D}} = T_z + \boxed{V_0^{1\mathrm{D}}(z)} \qquad V_{\mathrm{ext}}(z,t) = z \cdot \mathcal{E}_z(t)$$

Construction of the density-based 1D model potential

- Key idea:

$$\varrho_z^{100}(z) = 2\pi \int_0^\infty |\psi_{100}(z,\rho)|^2 \rho \mathrm{d}\rho$$
$$= \frac{\mu Z}{2} \left(2Z\mu|z| + 1\right) e^{-2Z\mu|z|}$$

$$\psi_0(z) = \sqrt{\frac{\mu Z}{2}} \sqrt{2\mu Z|z| + 1} e^{-\mu Z|z|}$$

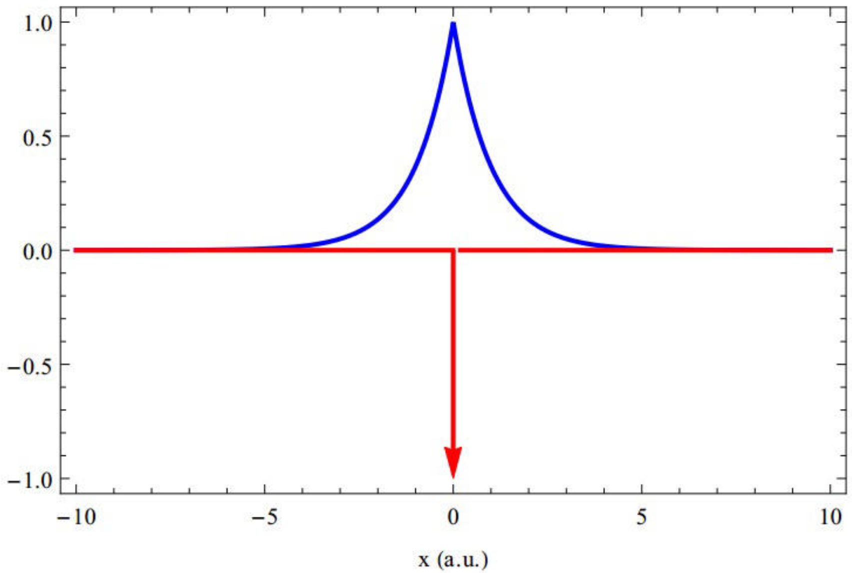
Construction of the density-based 1D model potential

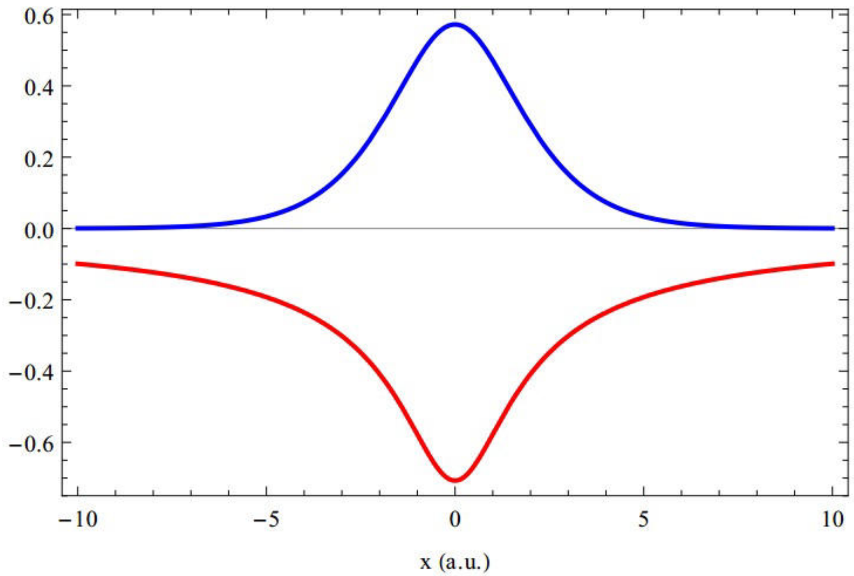
$$V_{0,\mathrm{M}}^{\mathrm{1D}}(z) = E_{0,\mathrm{M}} + \frac{1}{\psi_0(z)} \frac{1}{2\mu} \frac{\partial^2}{\partial z^2} \psi_0(z)$$

$$\lim_{|z|\to\infty} V_{0,\mathrm{M}}^{\mathrm{1D}}(z) = 0 \qquad E_{0,\mathrm{M}} = E_0 = -\frac{\mu Z^2}{2}$$

$$V_{0,\mathrm{M}}^{\mathrm{1D}}(z) = -\frac{1}{2\mu} \frac{1}{2^2 \left(|z| + \frac{1}{2\mu Z}\right)^2} - \frac{\frac{1}{2} Z}{|z| + \frac{1}{2\mu Z}}$$

Conventional 1D model potentials





$$V_D = \delta(x)$$

$$\Psi(x) = e^{-|x|}$$

$$E = -\frac{1}{2}$$

$$V_C = -\frac{1}{\sqrt{x^2+2}}$$

$$\Psi(x) = N e^{-\sqrt{x^2+2}}\left(1+\sqrt{x^2+2}\right)$$

$$E = -\frac{1}{2}$$

Improved 1D model potentials

- Improved soft-core Coulomb potential:

$$V_{0,\mathrm{M,Sc}}^{\mathrm{1D}}(z) = -\frac{\frac{1}{2}Z}{\sqrt{z^2 + \frac{1}{4Z^2}}} \qquad E_{0,\mathrm{M,Sc}} = -\frac{Z^2}{2}$$

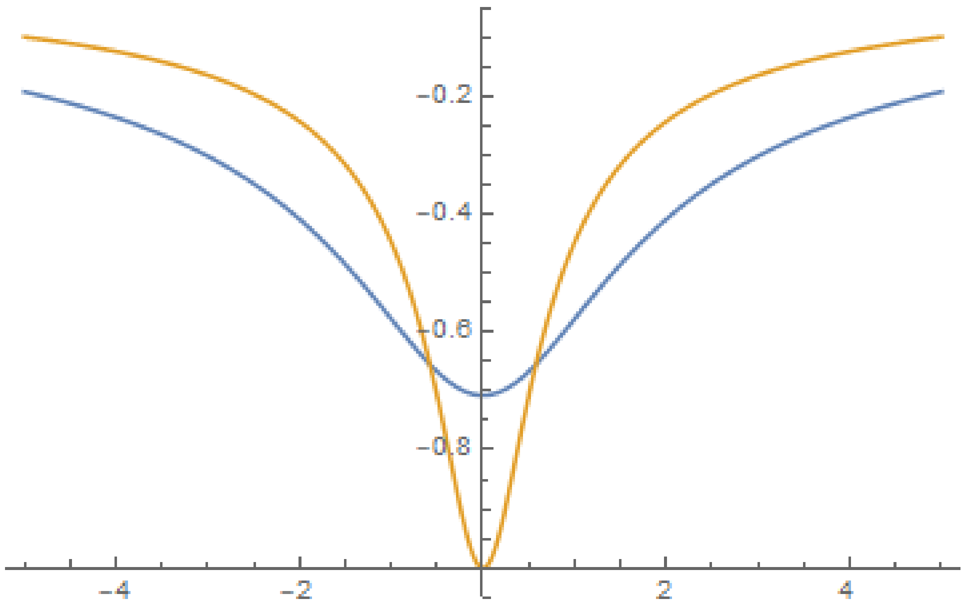
- Improved regularized Coulomb potential:

$$V_{0,\mathrm{M,C}}^{\mathrm{1D}}(z) = -\frac{\frac{1}{2}Z}{|z| + a} \qquad a \approx 0.32889$$

Improved 1D model potentials

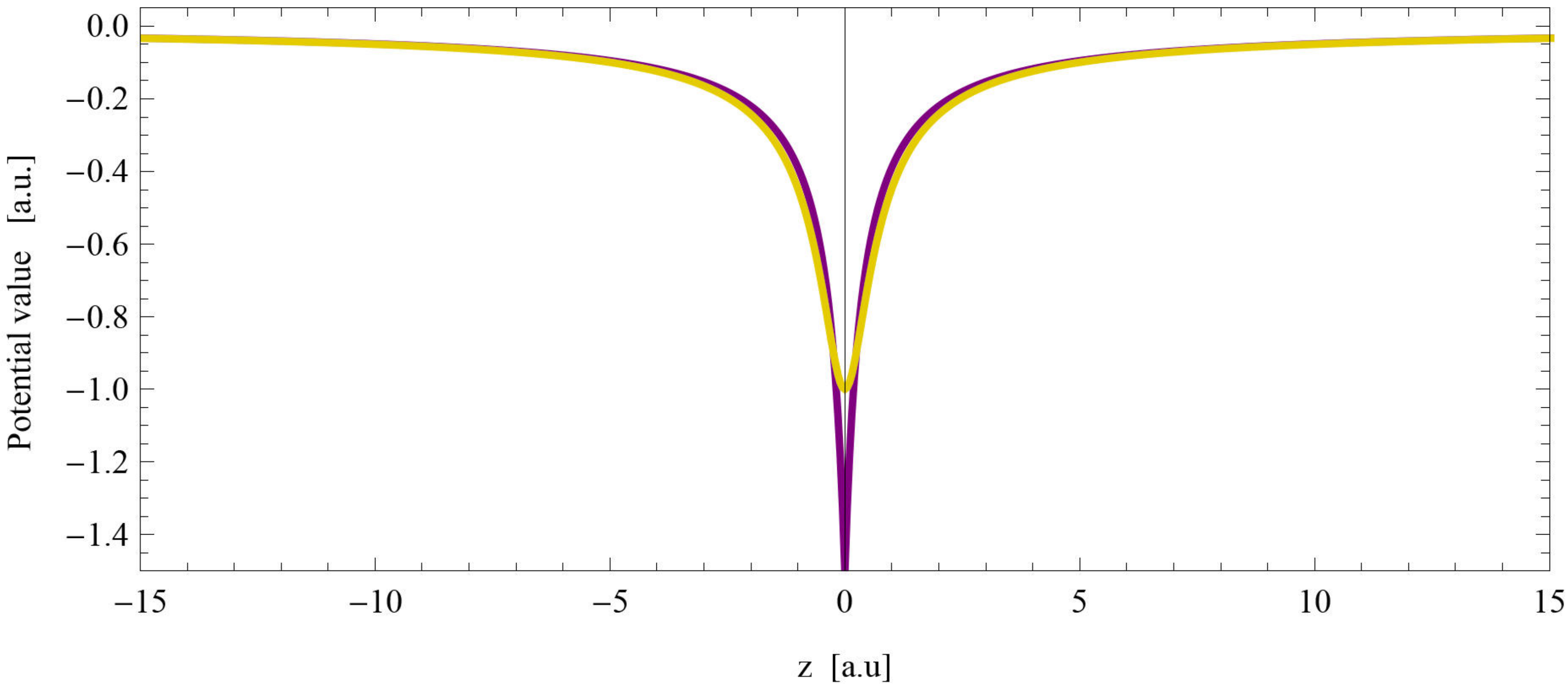
- Improved soft-core Coulomb potential:

$$V_{0,\mathrm{M},\mathrm{Sc}}^{1\mathrm{D}}(z) = -\frac{\frac{1}{2}Z}{\sqrt{z^2 + \frac{1}{4Z^2}}} \qquad E_{0,\mathrm{M},\mathrm{Sc}} = -\frac{Z^2}{2}$$



Improved 1D model potentials

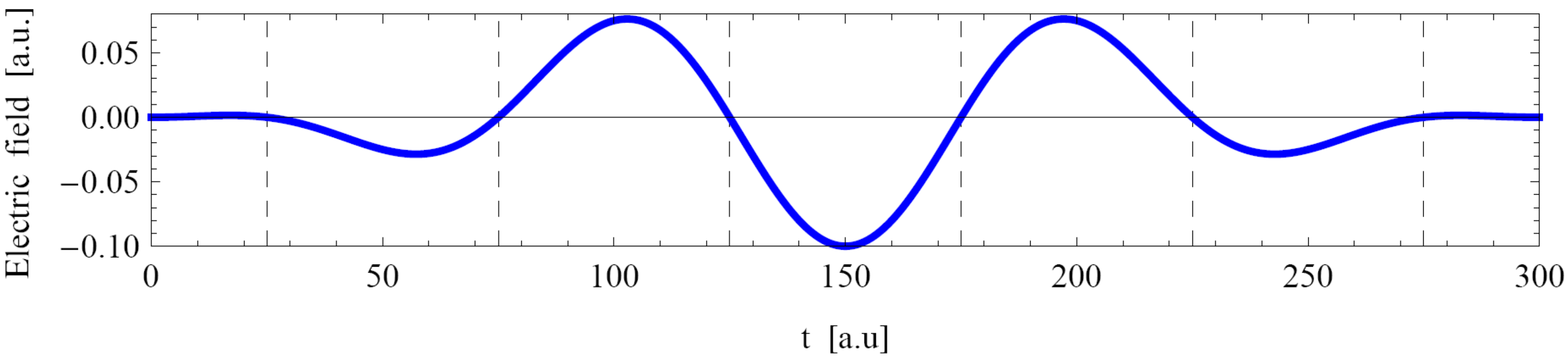
- Improved soft-core Coulomb potential vs. Density based model potential:



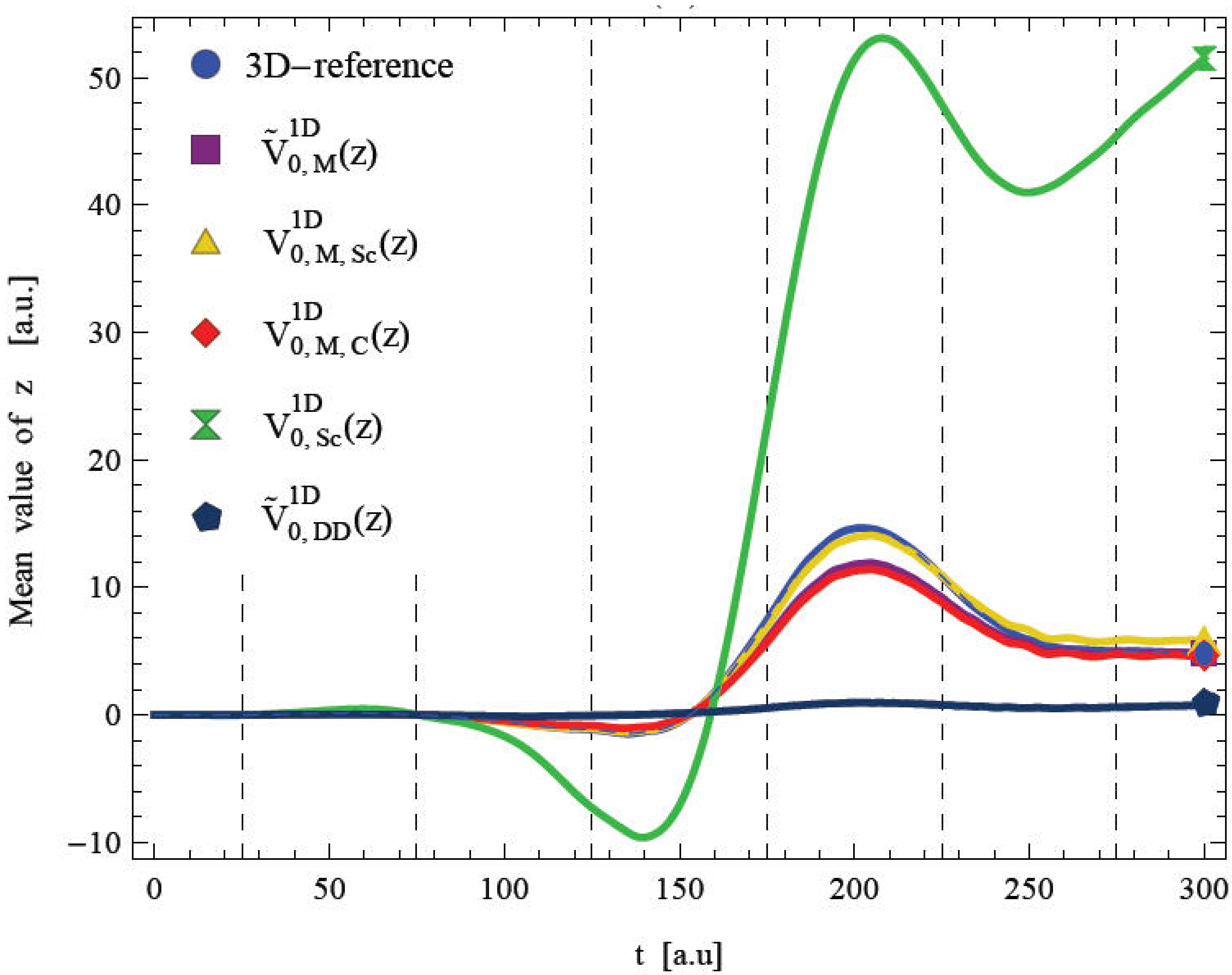
Simulation results

- Laser pulse:

$$\mathcal{E}_z(t) = F \cdot \sin^2\left(\frac{\pi t}{2N_{\text{Cycle}}T}\right)\cos\left(\frac{2\pi t}{T}\right)$$



Simulation results



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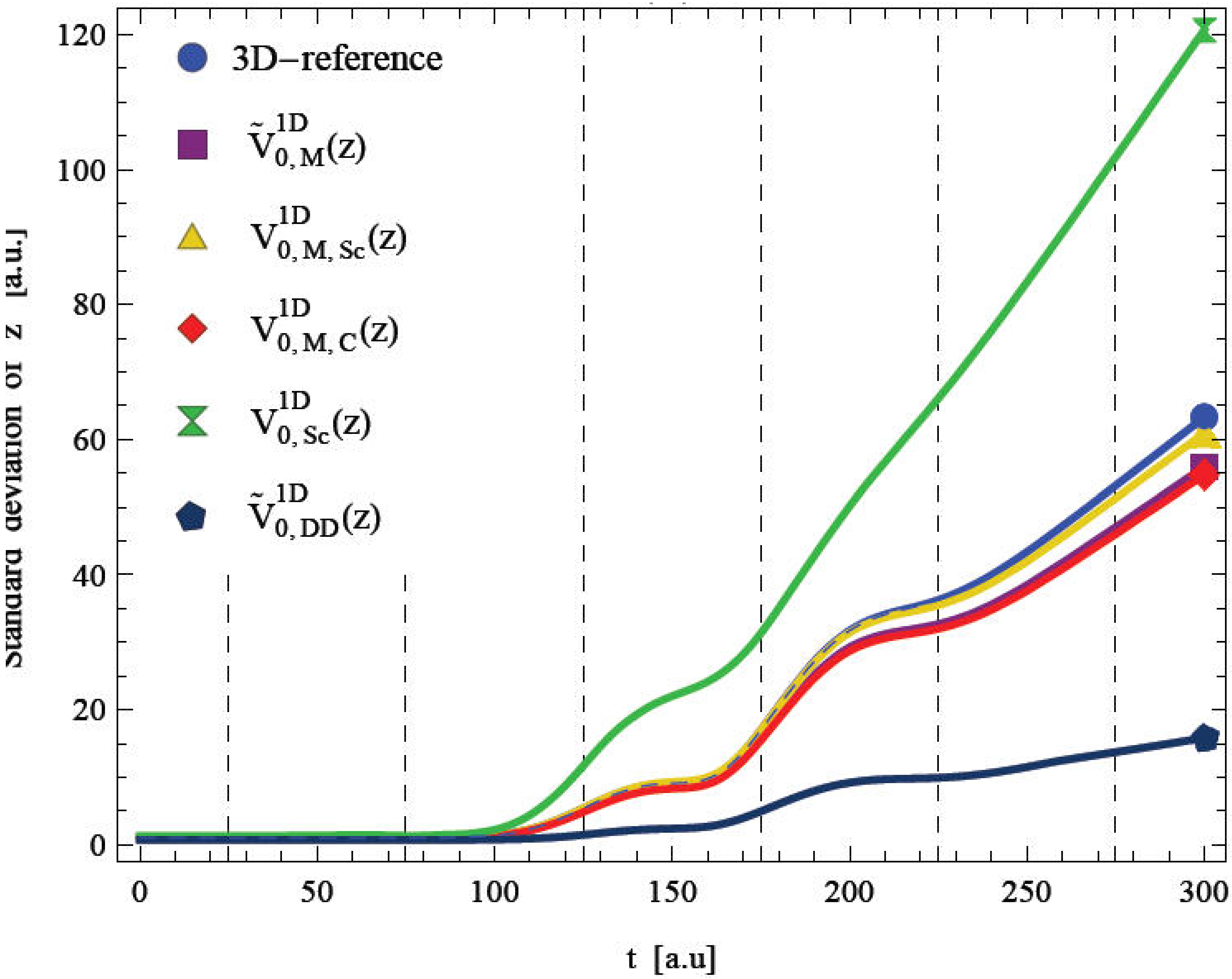

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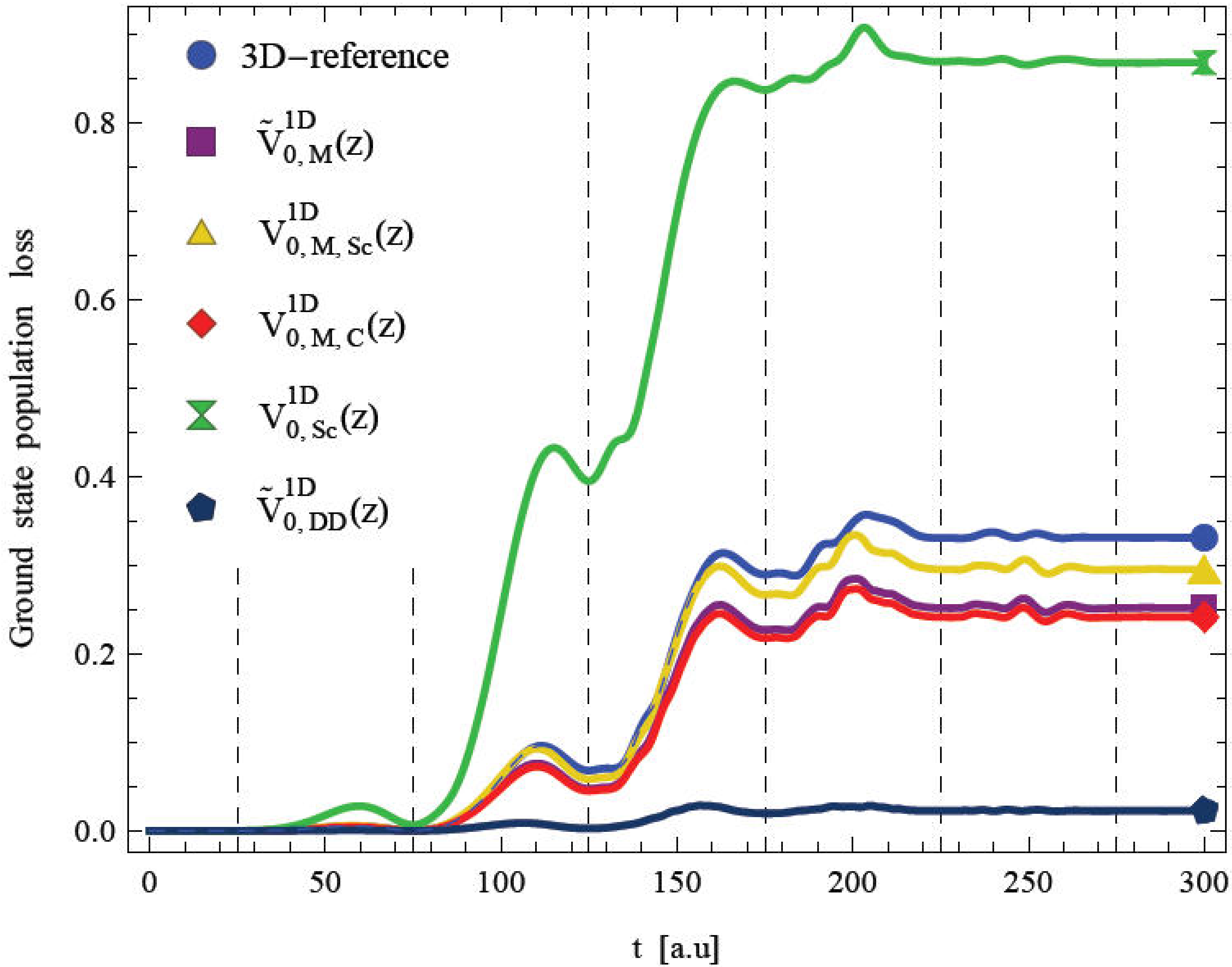

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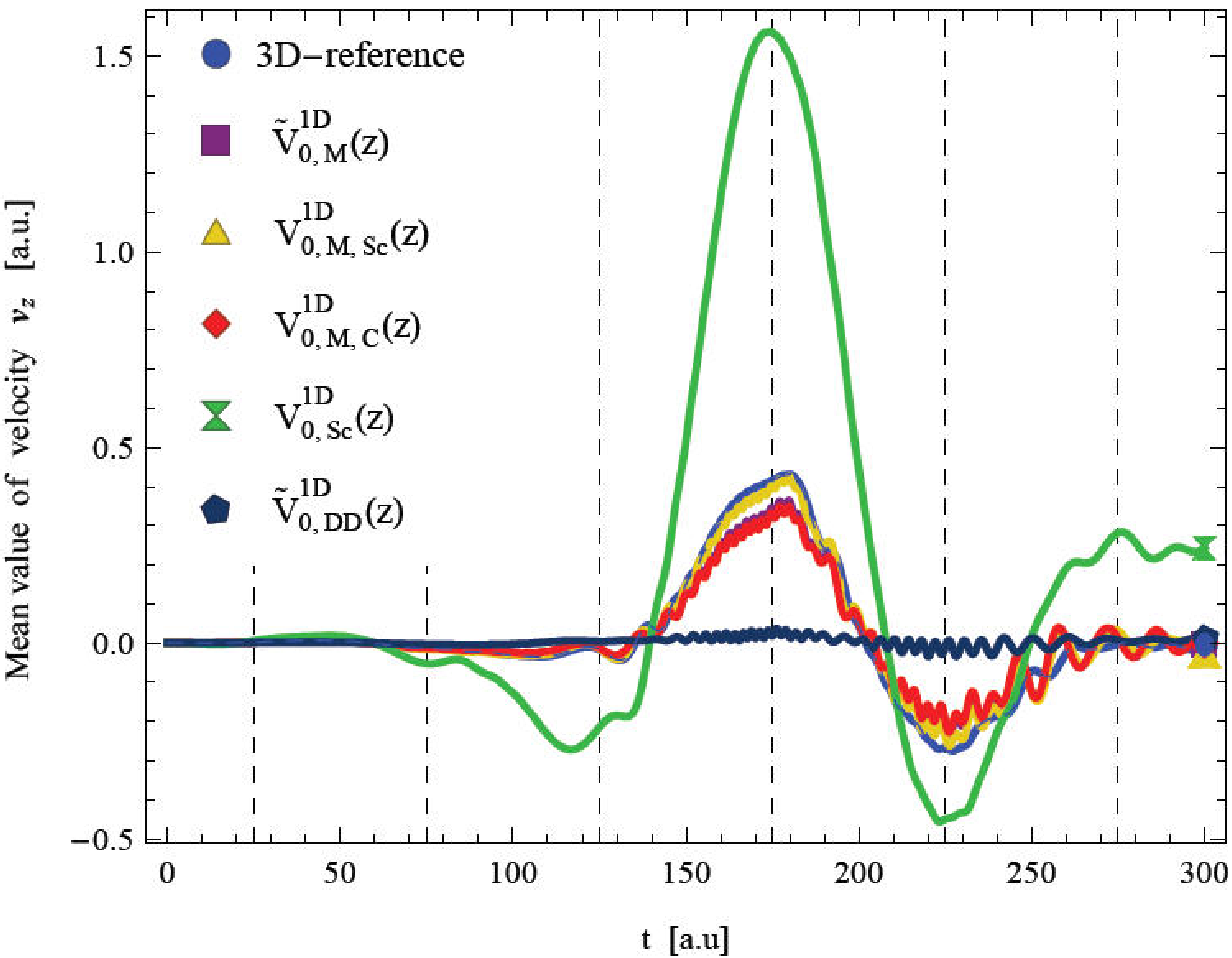

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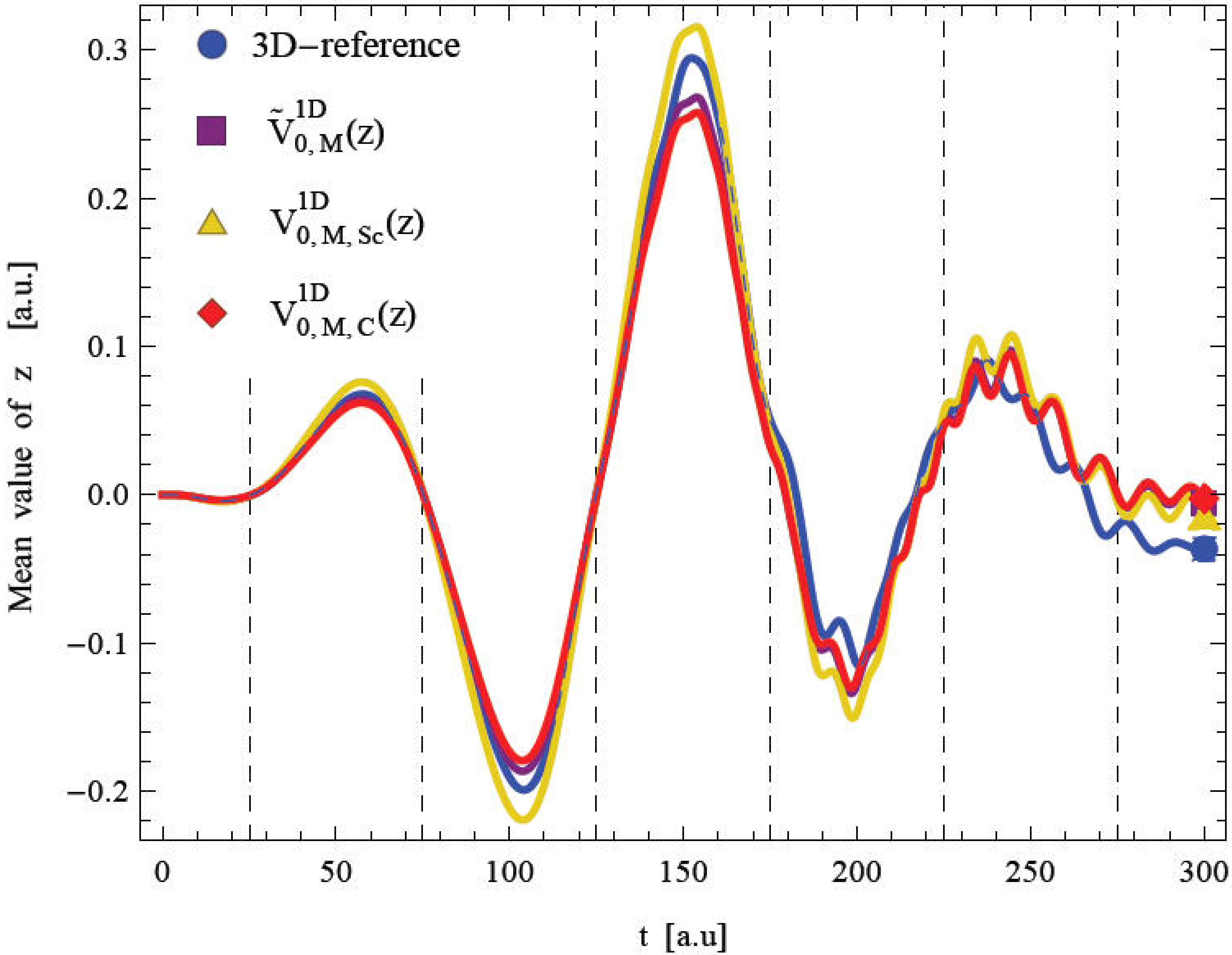

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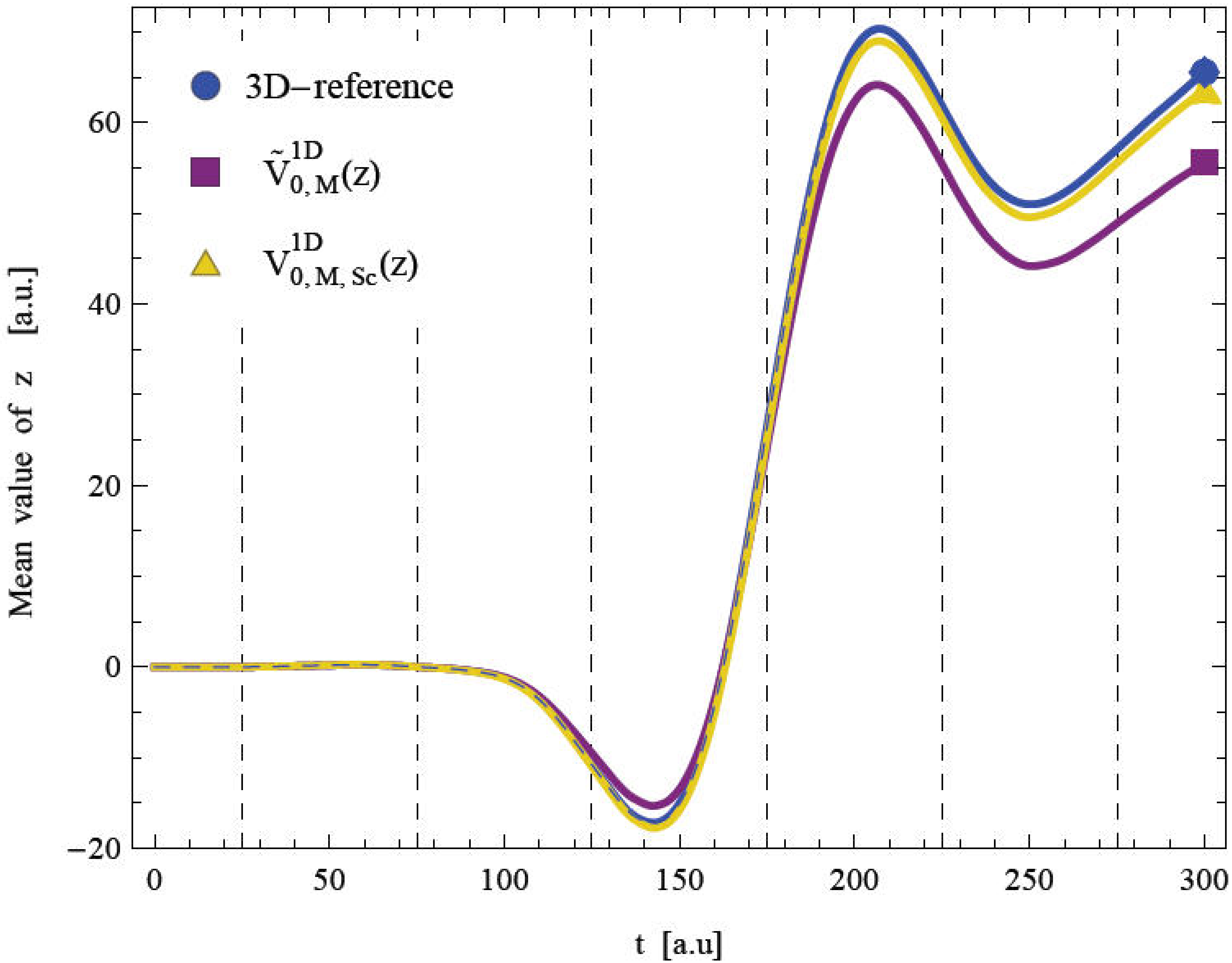

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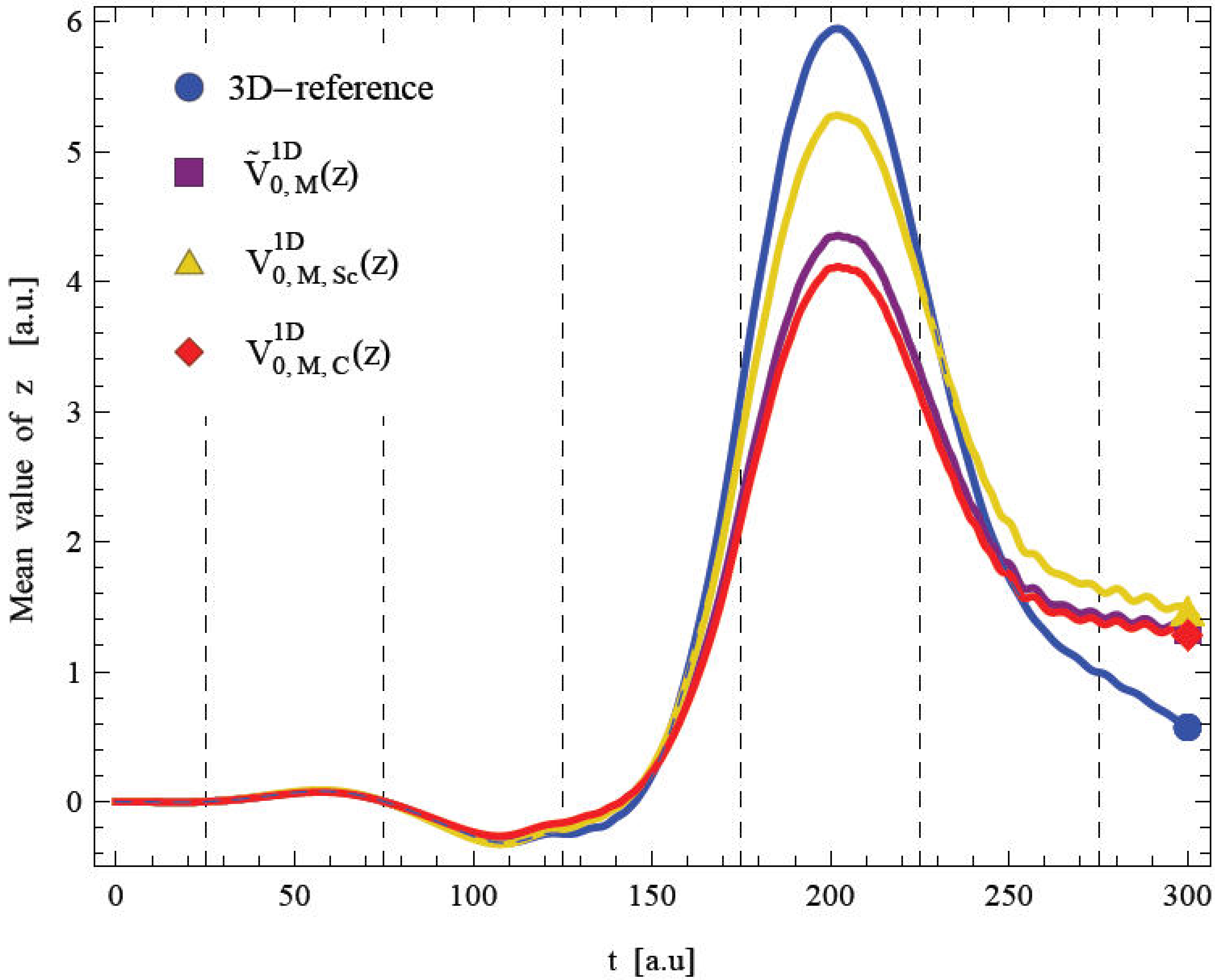

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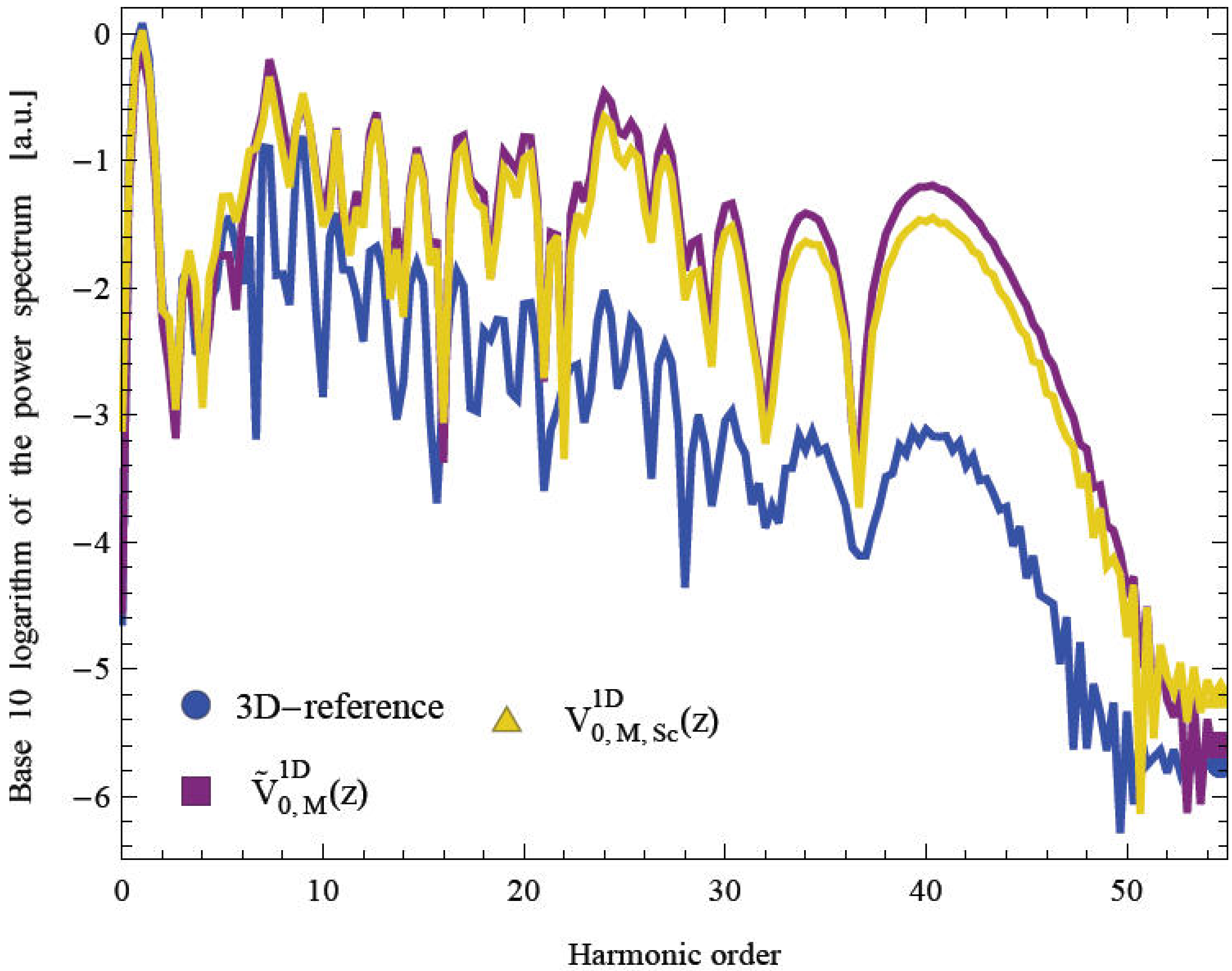

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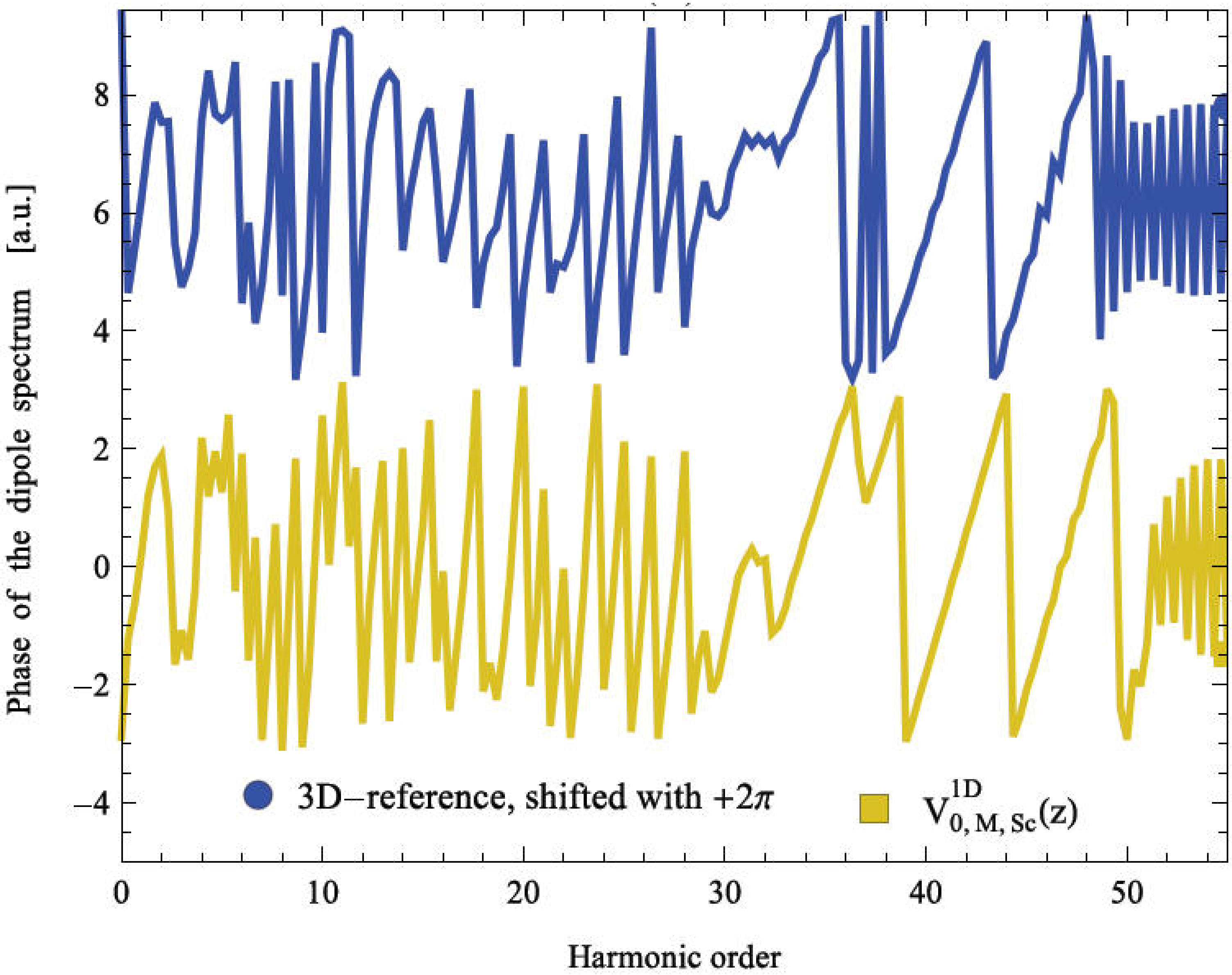

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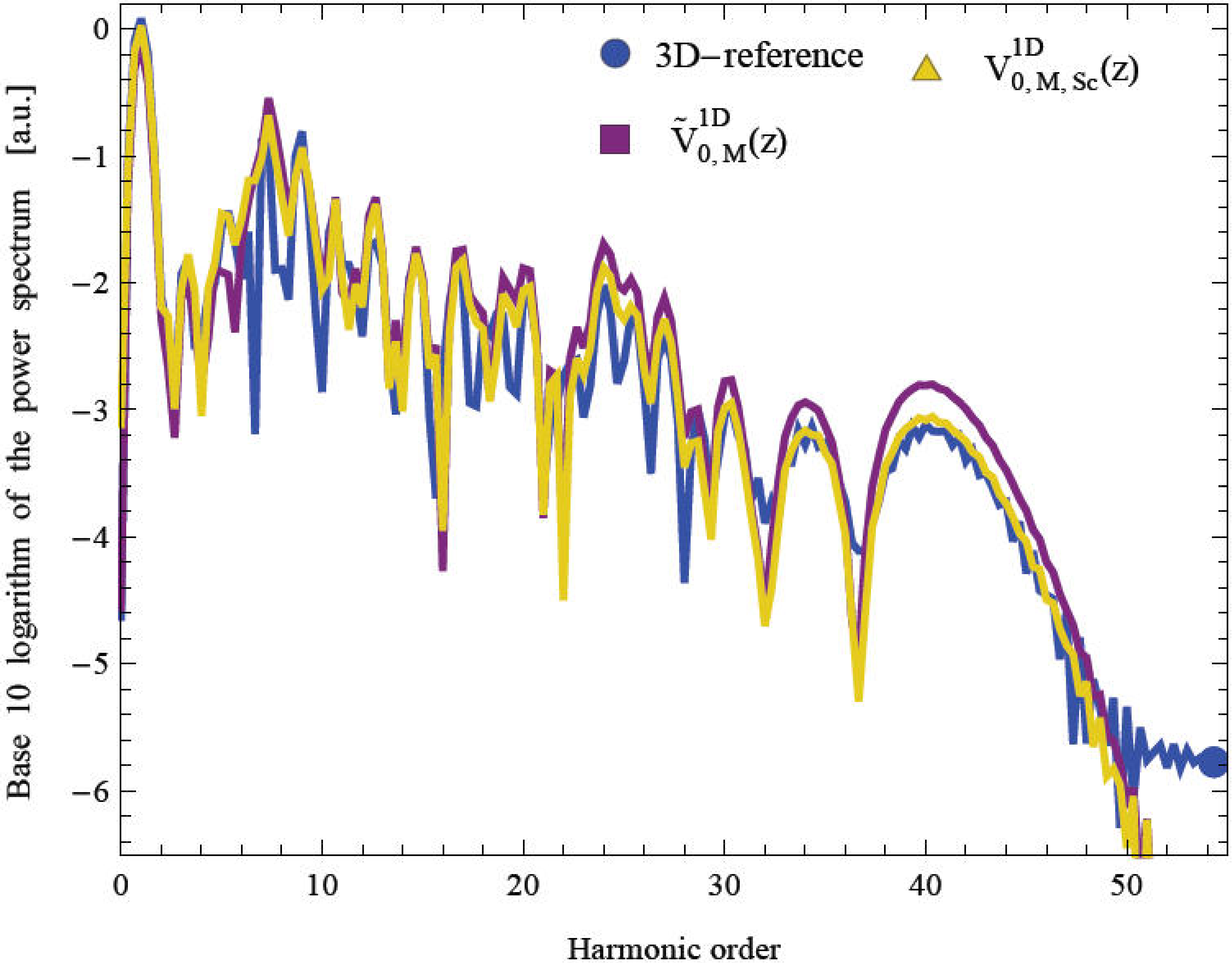

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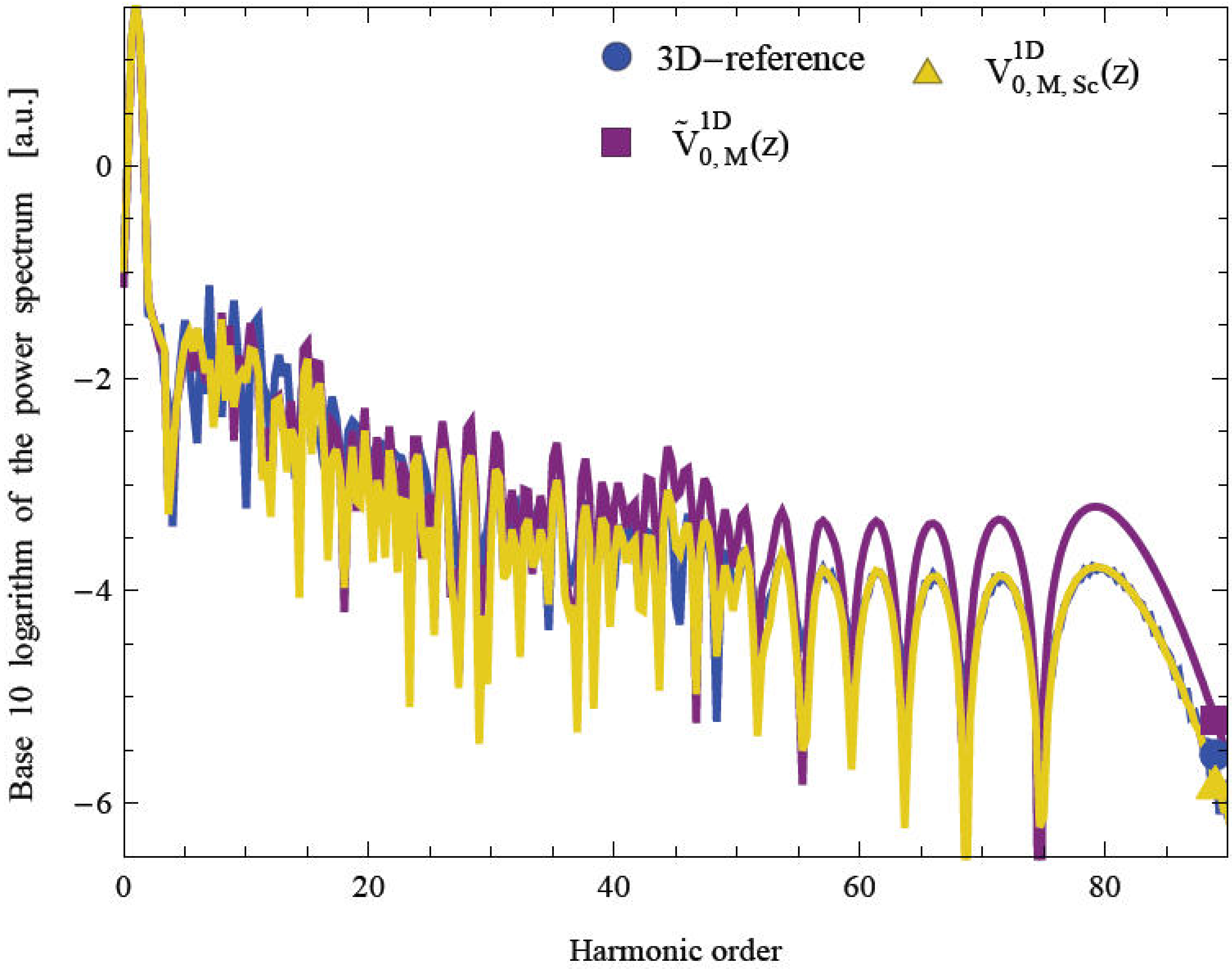

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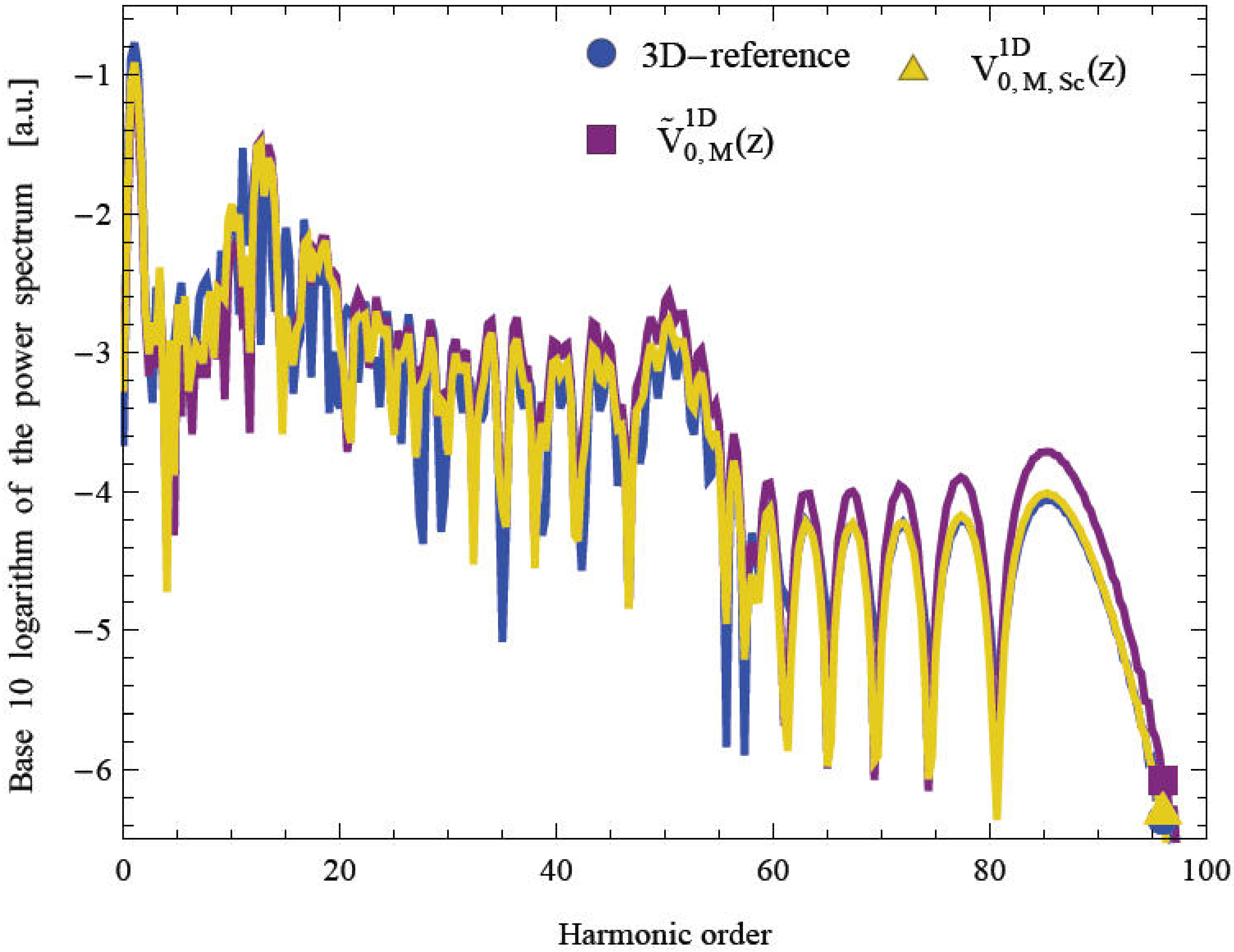

Conclusions

- The key idea leads to improved 1D model potentials
- Much more accurate low frequency results
- HHG spectra can be simply transformed to fit 3D results
- Future plans: 1D model potentials for He, H_2, H_2+

S. Majorosi, M. G. Benedict and A. Czirják, **arXiv:1806.03119**

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THANK YOU FOR YOUR ATTENTION!

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