

Typo Corrections: Physics-Informed Neural Networks for Quantum Propagators in Wavepacket Dynamics

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I. TYPO CORRECTIONS

1. Position: Page 13, Fig. 7

Published version:

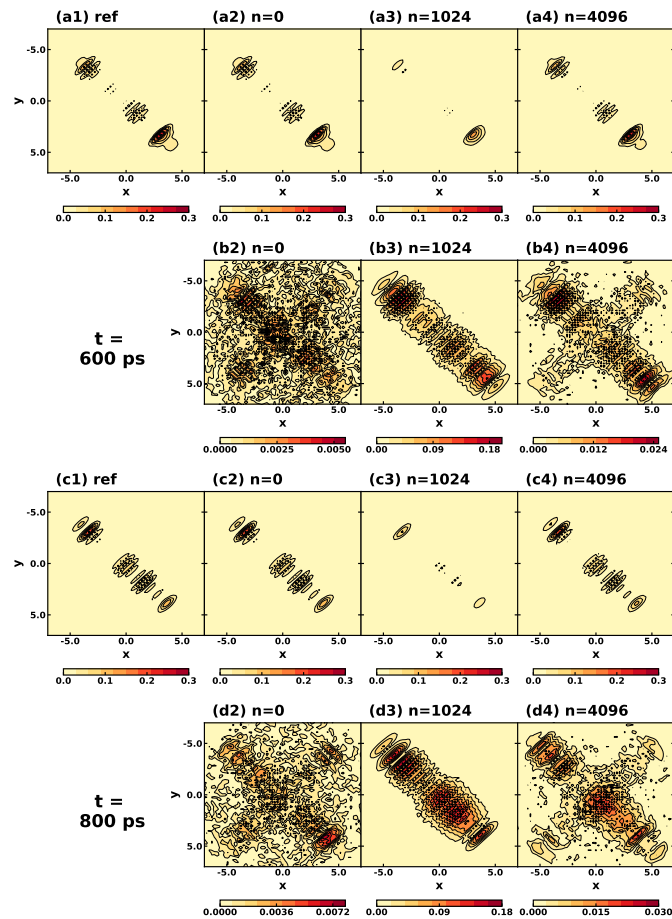


FIG. 1. Wavepacket dynamics of cross quadratic model (CQ) at zero temperature. (a) Probability distributions $|\psi(x,y)|^2$ at $t = 600$ au of reference dynamics (SOFT) and predicted dynamics by FCNs without hidden layer ($n = 0$) and different hidden sizes $n = 1024$ and 4096 , and (b) deviation the predicted wavepacket at $t = 600$ au, characterized by $|\psi^{\text{ref}}(x,y) - \psi^{\text{pred}}(x,y)|$. (c) Probability distributions $|\psi(x,y)|^2$ and (d) deviation of the predicted wavepacket at $t = 800$ au.

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Corrected:

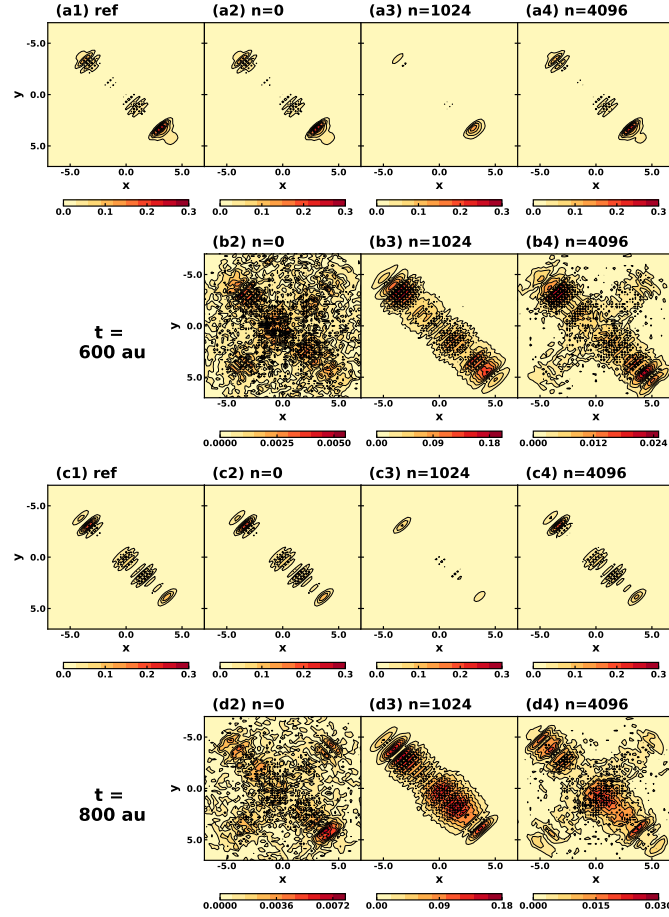


FIG. 2. Wavepacket dynamics of cross quadratic model (CQ) at zero temperature. (a) Probability distributions $|\psi(x,y)|^2$ at $t = 600$ au of reference dynamics (SOFT) and predicted dynamics by FCNs without hidden layer ($n = 0$) and different hidden sizes $n = 1024$ and 4096 , and (b) deviation the predicted wavepacket at $t = 600$ au, characterized by $|\psi^{\text{ref}}(x,y) - \psi^{\text{pred}}(x,y)|$. (c) Probability distributions $|\psi(x,y)|^2$ and (d) deviation of the predicted wavepacket at $t = 800$ au.

Comment: The time unit in the figure was wrong.

2. **Position:** Page 14, Fig. 8

Published version:

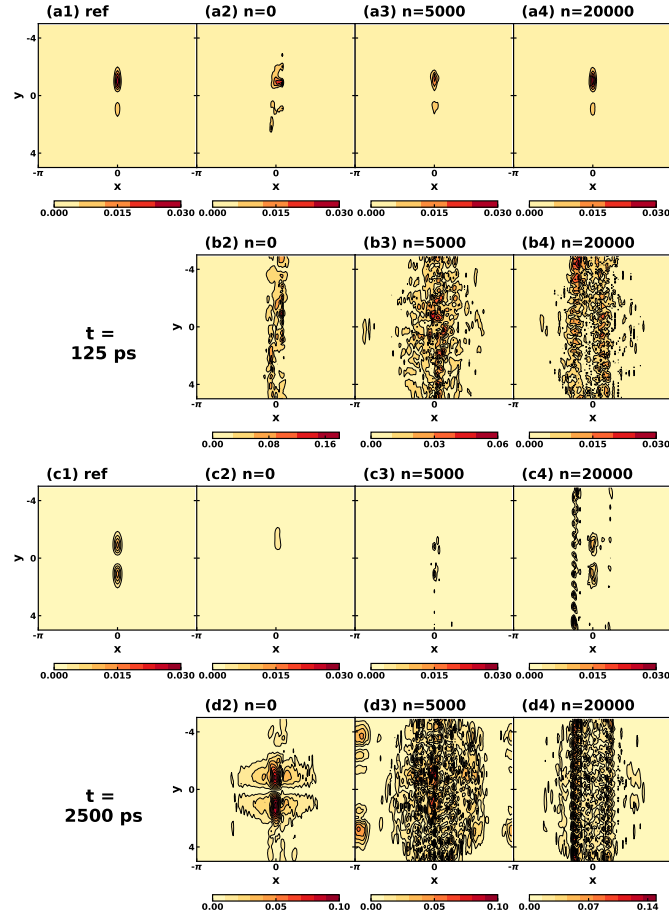


FIG. 3. Wavepacket dynamics of retinal model at zero temperature. (a) Probability distributions $|\psi_0(\varphi, q_c)|^2$ of the ground state at $t = 125$ au of reference dynamics (SOFT) and predicted dynamics by FCNs without hidden layer ($n = 0$) and different hidden sizes $n = 5000$ and 20000 , and (b) deviation the predicted wavepacket at $t = 125$ ps, characterized by $|\psi_0^{\text{ref}}(\varphi, q_c) - \psi_0^{\text{pred}}(\varphi, q_c)|$. (c) Probability distributions $|\psi_0(\varphi, q_c)|^2$ and (d) deviation of the predicted wavepacket at $t = 2500$ ps.

Corrected:

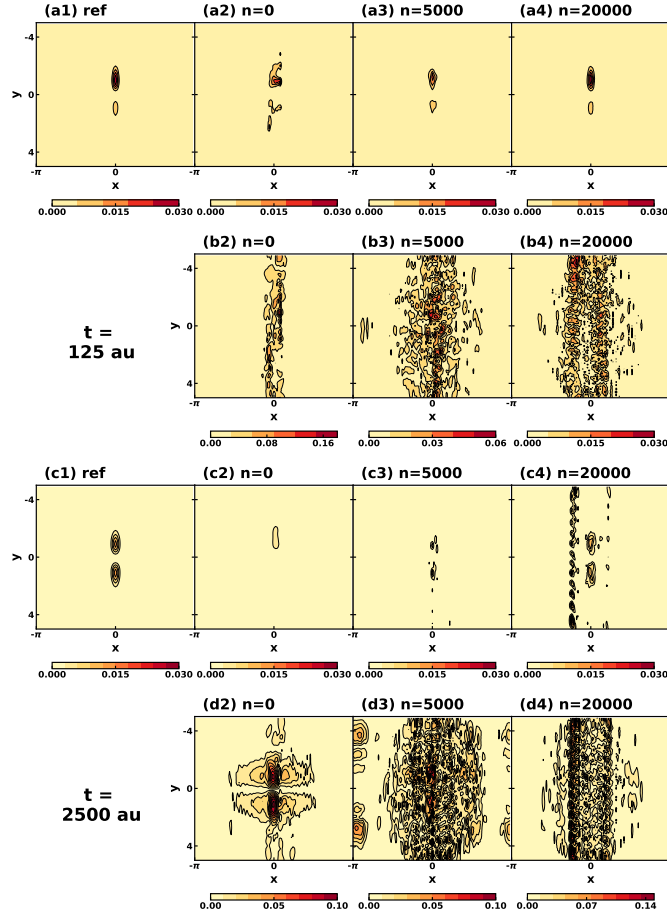


FIG. 4. Wavepacket dynamics of retinal model at zero temperature. (a) Probability distributions $|\psi_0(\varphi, q_c)|^2$ of the ground state at $t = 125$ au of reference dynamics (SOFT) and predicted dynamics by FCNs without hidden layer ($n = 0$) and different hidden sizes $n = 5000$ and 20000 , and (b) deviation the predicted wavepacket at $t = 125$ au, characterized by $|\psi_0^{\text{ref}}(\varphi, q_c) - \psi_0^{\text{pred}}(\varphi, q_c)|$. (c) Probability distributions $|\psi_0(\varphi, q_c)|^2$ and (d) deviation of the predicted wavepacket at $t = 2500$ au.

Comment: The time unit in the figure and caption was wrong.

3. **Position:** Page 15, Paragraph 2

Published version: ... For the CQ model, both the FCN without hidden layers and the one with $n = 4096$ achieve accurate predictions at time 600 ps and 800 ps, maintaining a relative error of approximately 1%. ...

Corrected: ... For the CQ model, both the FCN without hidden layers and the one with $n = 4096$ achieve accurate predictions at time 600 au and 800 au, maintaining a relative error of approximately 1%. ...

Comment: The time unit was wrong.

4. **Position:** Page 15, Paragraph 3

Published version: These limitations become even more pronounced in the 2D2S retinal model, where all tested FCNs fail to predict long-term dynamics up to 2500 ps even with a large hidden layer of size $n = 20000$

Corrected: These limitations become even more pronounced in the 2D2S retinal model, where all tested FCNs fail to predict long-term dynamics up to 2500 au even with a large hidden layer of size $n = 20000$

Comment: The time unit was wrong.