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Lattice Wigner Model

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Wigner Formulation

Wigner equation:

$$\frac{\partial w}{\partial t} + v\frac{\partial w}{\partial x} + \Theta[V]w = 0$$

Where:

$$(\Theta[V]w)(x,v,t) = -\sum_{\lambda} \frac{(\hbar/2i)^{\lambda-1}}{m^{\lambda}} \frac{1}{\lambda!} \frac{\partial^{\lambda} V}{\partial x^{\lambda}} \frac{\partial^{\lambda} w}{\partial v^{\lambda}}$$

Equivalent to Schrödinger

Why is it useful?

$$\frac{\partial w}{\partial t} + v\frac{\partial w}{\partial x} + \Theta[V]w = \Omega \longrightarrow$$

Open quantum systems

Lattice Wigner Model

Lattice Wigner equation:

$$W_i(\mathbf{x} + \mathbf{v}_i\delta t, t + \delta t) - W_i(\mathbf{x}, t) = \delta t\Omega_i + \delta t S_i +$$

$$\frac{\delta t}{2}\left(S_i(\mathbf{x}, t) - S_i(\mathbf{x} - \mathbf{v}_i\delta t, t - \delta t)\right)$$

$$\Omega_i = -\frac{1}{\tau_w}\left(W_i(\mathbf{x}, t) - W_i^{eq}(\mathbf{x}, t)\right) \longrightarrow \text{Numerical diffusion}$$

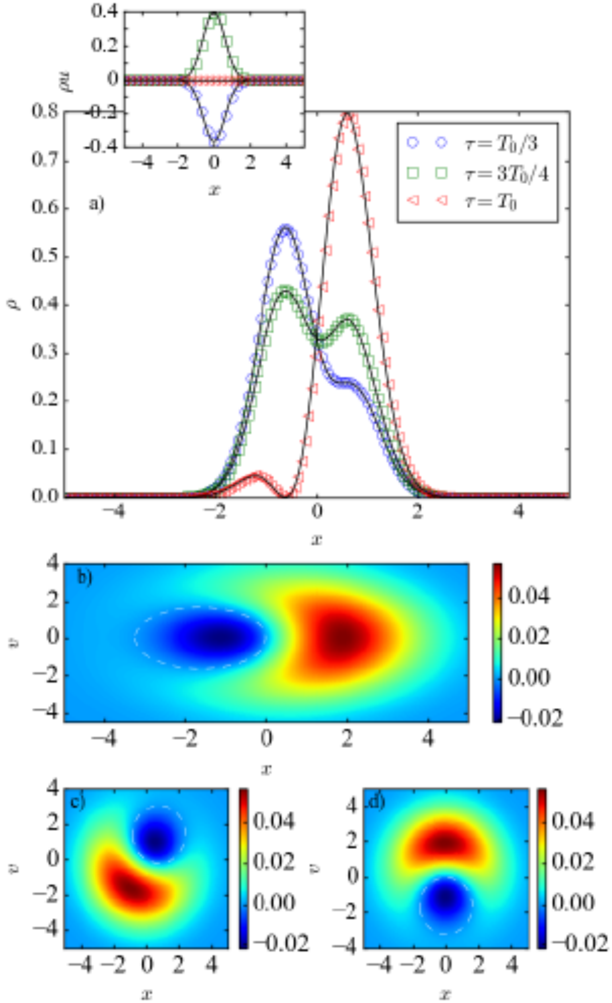
$$W_i = \omega_i \sum_n^{N_p} a_n(x,t)\mathcal{H}_n(v_i; c_s)$$

$$a_n(x,t) = \sum_i^N \bar{W}_i H_n(v_i; c_s)$$

$$\bar{W}_i^{eq} = \omega_i \sum_n^{N_\Pi} a_n(x,t)\mathcal{H}_n(v_i; c_s)$$

$$S_i = -\omega_i \sum_{n,s} a_n(x,t)\sqrt{\frac{(n+s)!}{n!}}\frac{(-H/i)^{s-1}}{c_s^s s!}\frac{\partial^s V}{\partial x^s}\mathcal{H}_{n+s}(v_i; c_s).$$

Lattice Wigner Model



$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{1}{2}\hat{x}^2$$

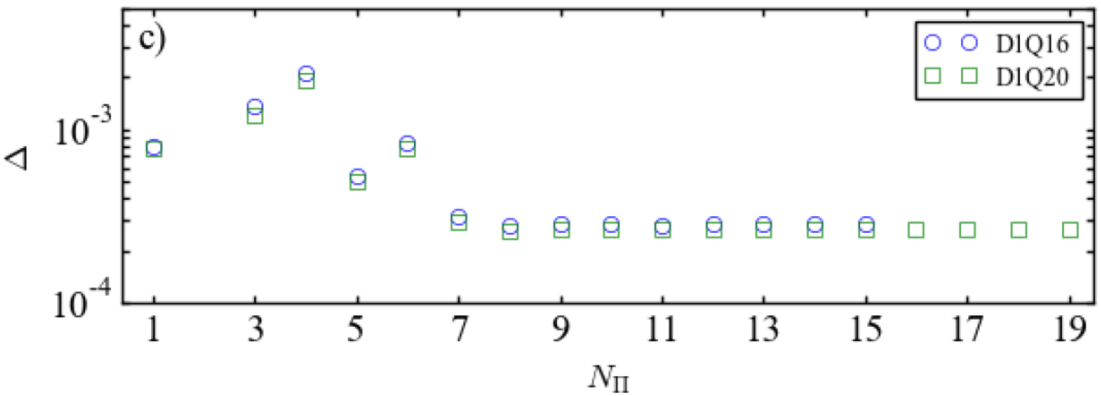
$$|\phi\rangle \;=\; \frac{1}{\sqrt{2}}(|\psi_0\rangle + |\psi_1\rangle)$$

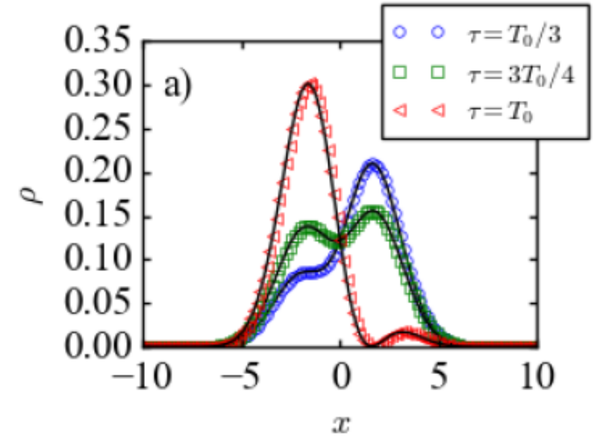
$$W_{|\phi\rangle}(x,v) = \frac{e^{-\frac{v^2+x^2}{H}}\left(\sqrt{2}\sqrt{H}x + v^2 + x^2\right)}{\pi H^2}$$

Harmonic oscillator

Lattice Wigner Model

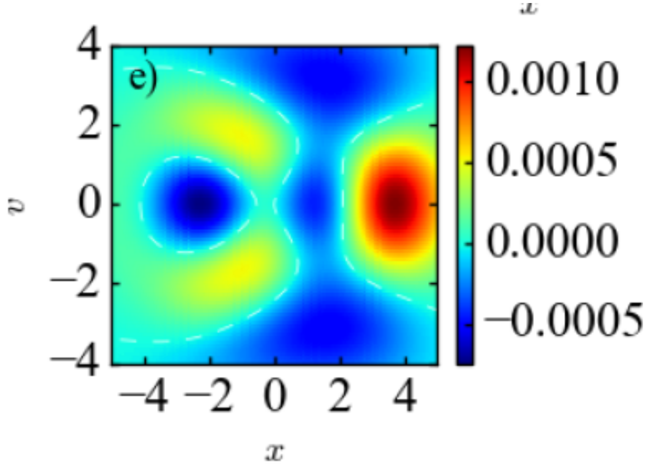
Error due to numerical diffusivity:





Anharmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{1}{2}\hat{x}^2 + \alpha\hat{x}^4 + \beta\hat{x}^6$$



Lattice Wigner Model

3D simulation of randomly located Gaussian potential barriers: