Obtaining complete quantum dynamics via a controlled extrapolation from semiclassical methods

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Quantum dynamics: THE ISSUE

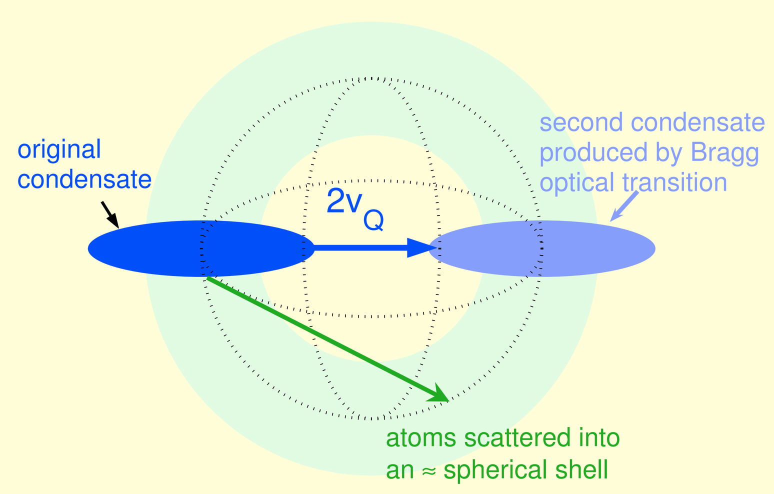
- COMPLETE METHODS – Intractable or run for a limited time. *(positive-P, stochastic wavefunction,…)*
- TRACTABLE METHODS – Incomplete (Sometimes appreciably, sometimes not). *(GP, PGPE, c-field,…)*

A (partial) Remedy

1. Suppose we have:
   (a) A complete method $\mathcal{Q}$ that is tractable only for a short time.
   (b) Approximate methods $\mathcal{A}$, $\mathcal{B}$, …that are tractable for long times.
2. Suppose $\mathcal{A}$ and $\mathcal{B}$ are similar enough to $\mathcal{Q}$ that an ad-hoc *continuous* blend of the evolution equations can be made:
   - $\mathcal{H}_{\mathcal{A}} = \lambda\mathcal{Q} + (1-\lambda)\mathcal{A}$
   - $\mathcal{H}_{\mathcal{B}} = \lambda\mathcal{Q} + (1-\lambda)\mathcal{B}$

   With blending parameter $\lambda \in [0,1]$. Here $\lambda \to 1$ as the equations approach full QD.
3. A judicious choice of hybrid evolution equations produces simulations that *last much longer than the exact method* $\mathcal{Q}$, but have *smaller systematics than* $\mathcal{A}$ *or* $\mathcal{B}$.
4. With λ continuous, one can extrapolate to $\lambda = 1$ obtain an estimate of the full quantum mechanical result.
5. With two different hybrids $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$, wild extrapolations are prevented.
6. The uncertainty of the final predictions can be well characterised from their statistics.

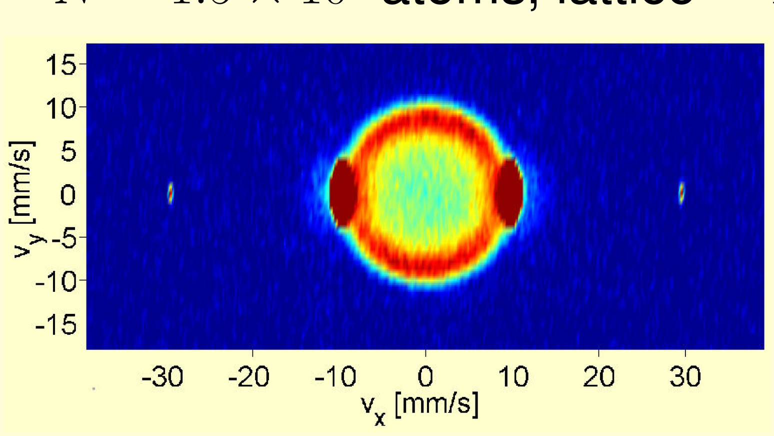
Example: BEC collision



Some experiments:

- He^* A.Perrin et al., PRL 99, 150405 (2007).
- Na A.P.Chikkatur et al, PRL 85, 483 (2007). J.M.Vogels et al, PRL 89, 020401 (2007).
- Rb N.Katz, PRL 95, 220403 (2005).

$N = 1.5\times 10^5$ atoms, lattice $\sim 10^6$ points.



Na

positive-P

PD&P.D.Drummond, PRL 98,120402 (2007)

$\mathcal{Q}$: Complete dynamics: Positive P distribution

Random walk of samples $\psi(x)$ and $\tilde{\psi}(x)$

[Equivalent to full QD in the ∞ samples limit.]

$$i\hbar\frac{d\psi(x)}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + g\,\psi(x)\tilde{\psi}^*(x) + \sqrt{\frac{g}{i\hbar}}\,\xi(x,t)\right]\psi(x)$$

$$i\hbar\frac{d\tilde{\psi}(x)}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + g\,\psi(x)\tilde{\psi}^*(x) + \sqrt{\frac{-g}{i\hbar}}\,\tilde{\xi}(x,t)\right]\tilde{\psi}(x)$$

= mean field GP + noise fields $\xi, \tilde{\xi}$

$$\overline{n}(x) = \left\langle \widehat{\Psi}^\dagger(x)\widehat{\Psi}(x)\right\rangle = \left\langle \tilde{\psi}^*(x)\psi(x)\right\rangle_{\text{ensemble}}$$

$\mathcal{A}$: Truncated Wigner

GP evolution + $\frac{1}{2}$ virtual particle in IC

$$\psi(x,0) = \phi_{GP}(x,0) + \frac{\eta(x)}{\sqrt{2}} \qquad \eta(x): \text{gaussian noise}$$

$$i\hbar\frac{d\psi(x)}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + g\,|\psi(x)|^2\right]\psi(x)$$

$$\overline{n}(x) = \left\langle |\psi(x)|^2 - \frac{1}{2}\right\rangle_{\text{ensemble}}$$

$\mathcal{B}$: GP mean field

$\mathcal{H}_{\mathcal{A}}$: tWigner / +P blend

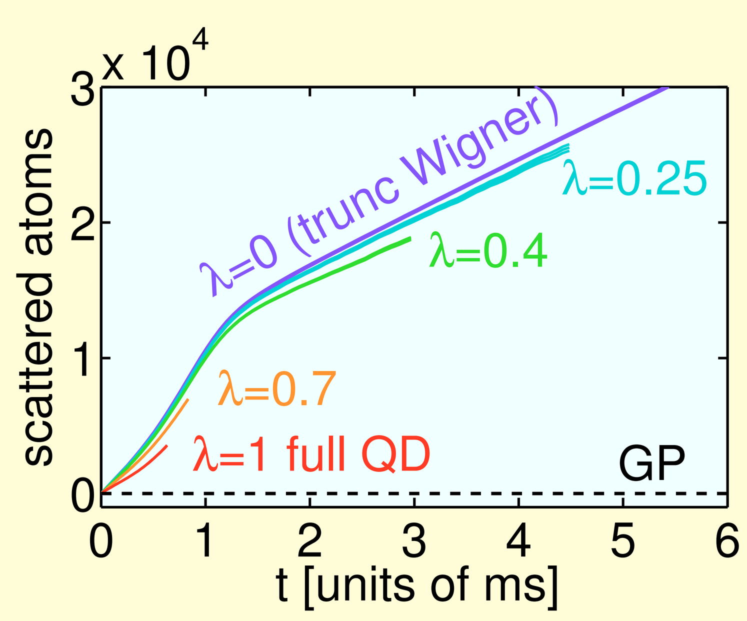
$\lambda = 0$: Wigner, $\lambda = 1$: complete QD

$$\psi(x,0) = \tilde{\psi}(x,0) = \phi_{GP}(x,0) + \sqrt{\frac{1-\lambda}{2}}\,\eta(x)$$

$$i\hbar\frac{d\psi(x)}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + g\,\psi(x)\tilde{\psi}^*(x) + \sqrt{\frac{\lambda g}{i\hbar}}\,\xi(x,t)\right]\psi(x)$$

$$i\hbar\frac{d\tilde{\psi}(x)}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + g\,\psi(x)\tilde{\psi}^*(x) + \sqrt{\frac{-\lambda g}{i\hbar}}\,\tilde{\xi}(x,t)\right]\tilde{\psi}(x)$$

$$\overline{n}(x) = \left\langle \tilde{\psi}^*(x)\psi(x) - \frac{1-\lambda}{2}\right\rangle_{\text{ensemble}}$$



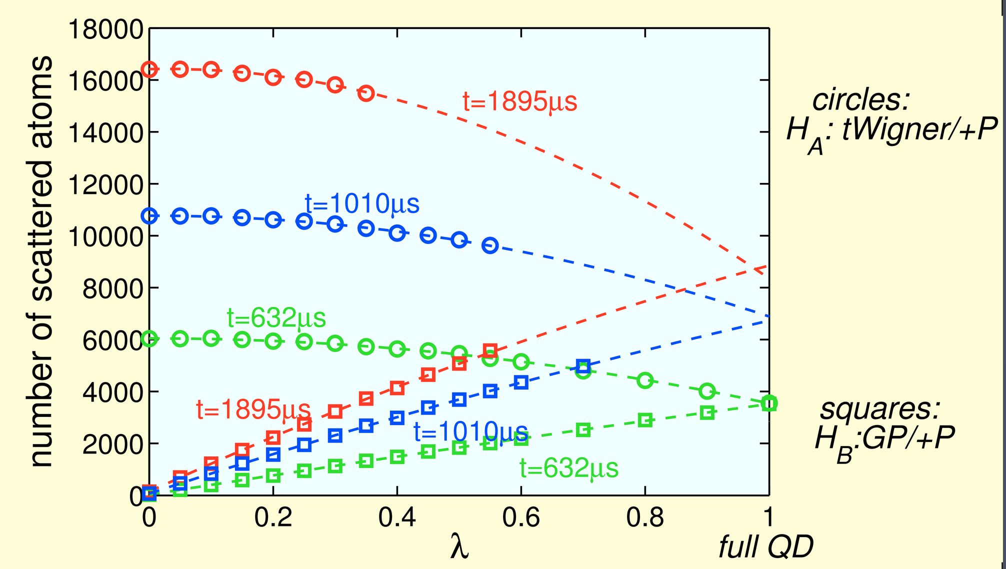
Bad features of both methods BUT STILL USEFUL

$\mathcal{H}_{\mathcal{B}}$: GP / +P blend

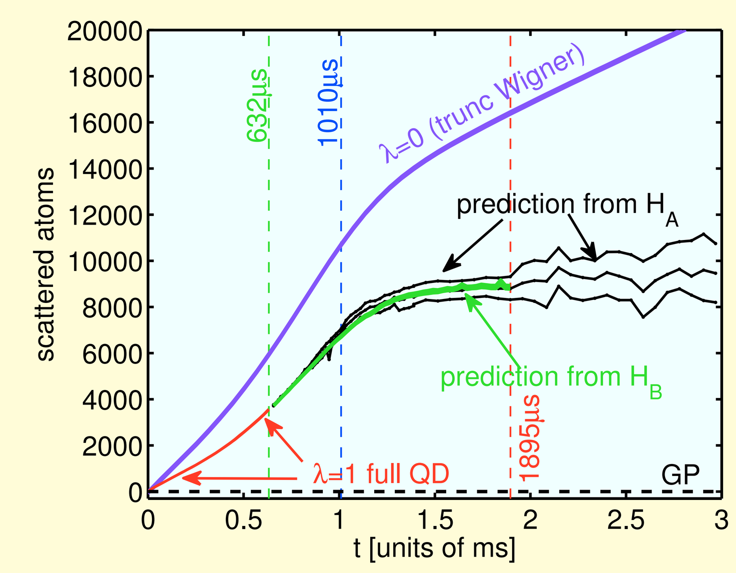
Identical to positive-P except noise is multiplied by $\sqrt{\lambda}$ as per $\sqrt{\frac{\lambda g}{i\hbar}}\,\xi(x,t)$, etc.

No. of halo scattered atoms

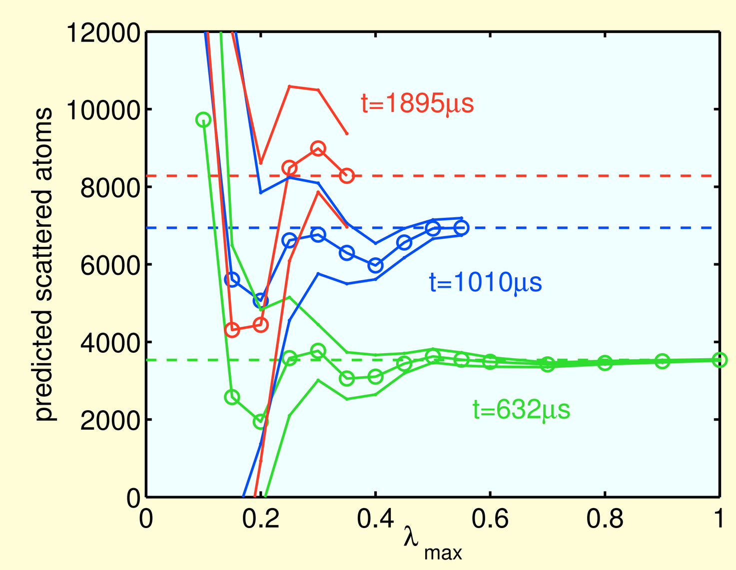
λ-EXTRAPOLATION:



FINAL PREDICTIONS: (1σ error bars)

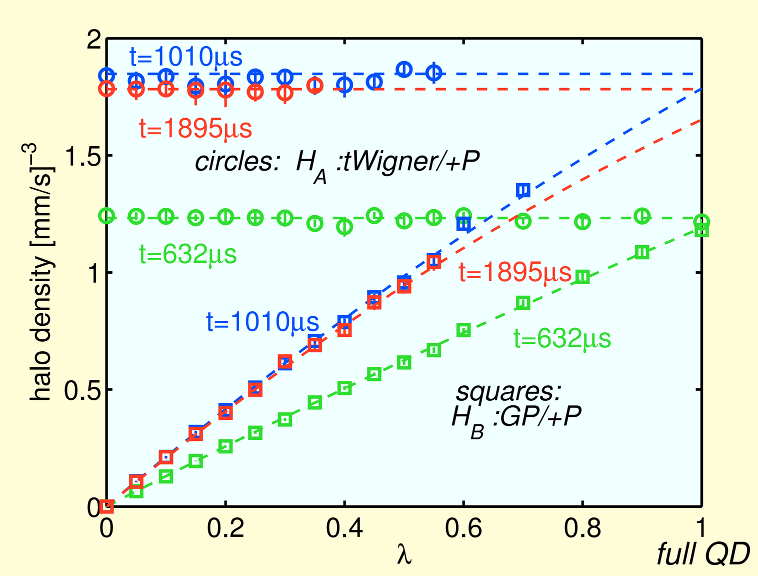


CHECK: EXTRAPOLATION USING A LIMITED λ RANGE $\lambda \in [0, \lambda_{\max}]$



Peak halo density

λ-EXTRAPOLATION:



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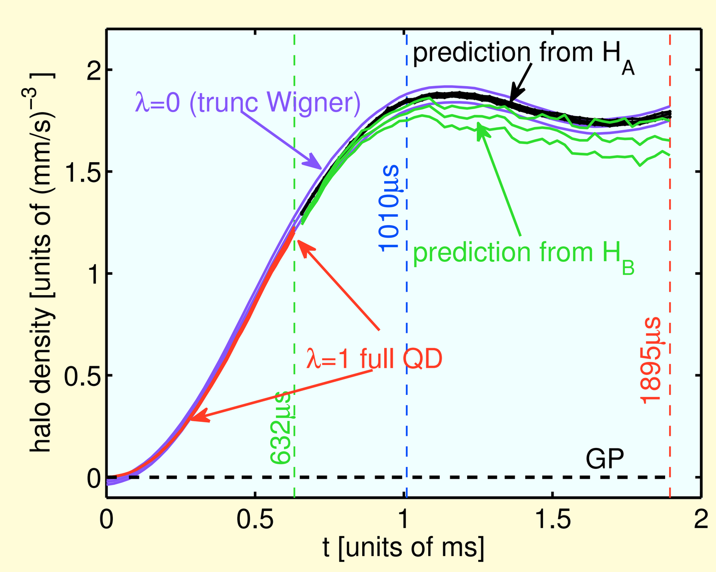

P. Deuar, arXiv:0903.1309, to appear in PRL.

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