A controlled transition
FROM: Classical field simulations
TO: Full quantum dynamics

Piotr Deuar

LPTMS
Université Paris-sud XI
Orsay, France

Thanks go to: Georgy Shlyapnikov (Orsay)
Peter Drummond (Univ. of Queensland)
Scott Hoffmann (Univ. of Queensland)

DAMOP, 29 May 2008

Classical field and positive P simulations

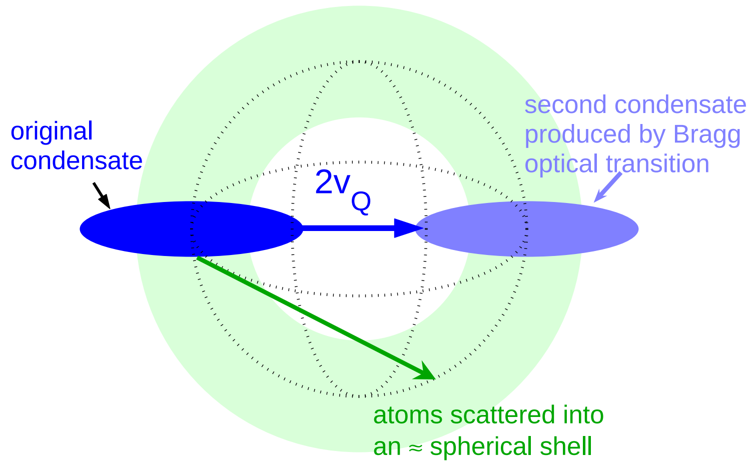
- Both give simulations of quantum dynamics beyond a linearised Hamiltonian
- Both are numerically tractable
- Each method has its drawbacks
- A hybrid method can alleviate some of these

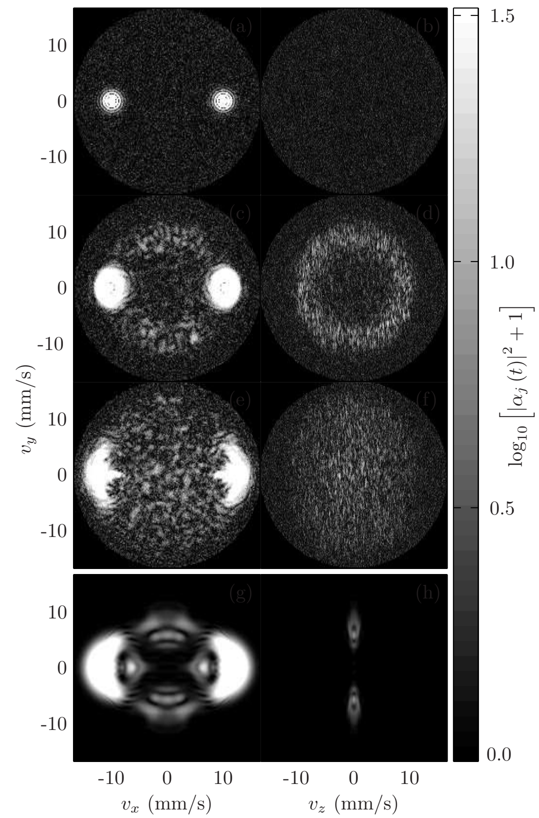
Classical field ("truncated Wigner") simulations

EXAMPLE SYSTEM: BEC COLLISION

Mean field fails for scattered atoms

x-space





CLASSICAL FIELD

k-space

[A.A. Norrie, R.J. Ballagh, & C. W. Gardiner, PRL **94**, 040401 (2005)]

MEAN FIELD

Experiments as per e.g.

[J. M. Vogels, K. Xu, & W. Ketterle, PRL **89**, 020401 (2002)]

and many others

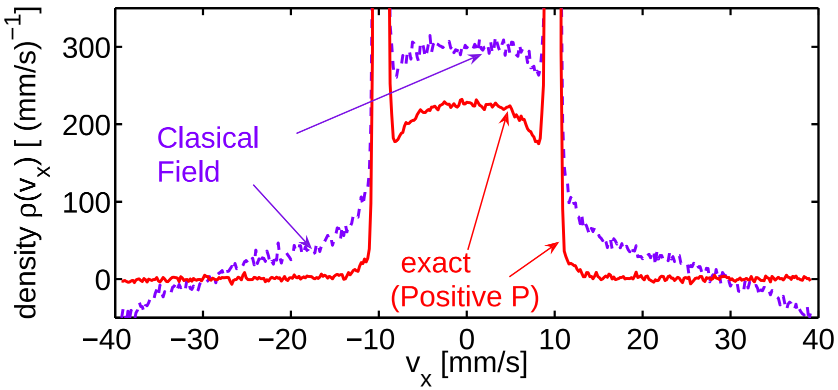
$$\psi(x,0) = \phi(x,0) + \frac{\eta(x)}{\sqrt{2}} \qquad \text{(add } \tfrac{1}{2} \text{ virtual particle)}$$

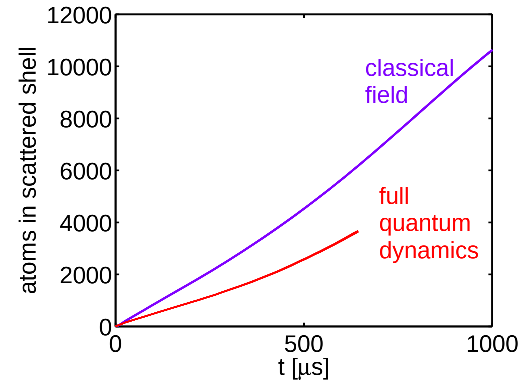
$$\widehat{H} = \mathrm{K.E.} + \frac{g}{2}\int \left[\widehat{\Psi}^\dagger(x)\right]^2 \widehat{\Psi}(x)^2 \, d^3x$$

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

Works well for large N= 6,000,000 particles

Less particles: N = 150,000



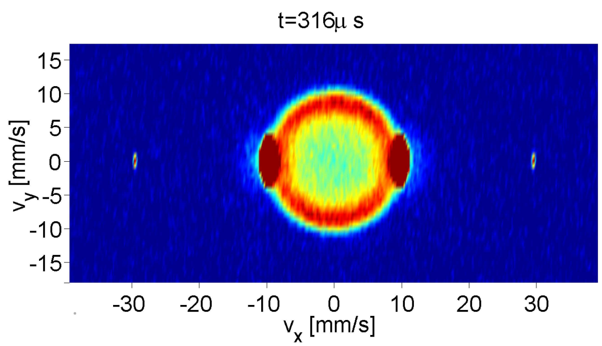


Full quantum dynamics (positive-P) calculations

$$\psi(x,0)=\phi(x,0) \quad ; \quad \tilde{\psi}(x,0)=\phi(x,0)$$

two fields

no virtual initial particles



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

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

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

mean field GP + noise

Classical field has errors for N= 150,000 particles

Positive P only works for short times

Hybrid representation

- Consruct a smooth transition parametrised by parameter λ
- $\lambda = 0$ is classical Field, $\lambda = 1$ is positive-P
- Want transition to be monotonic!

After some tries, obtain:

$$\psi(x,0) = \widetilde{\psi}(x,0) = \phi(x,0) + \sqrt{\frac{f_1(\lambda)}{2}}\eta(x)$$

initial conditions

$$i\hbar\frac{d\psi(x)}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + g\psi(x)\widetilde{\psi}^*(x) + f_2(\lambda)\sqrt{\frac{g}{i\hbar}}\,\xi(x,t)\right]\psi(x)$$

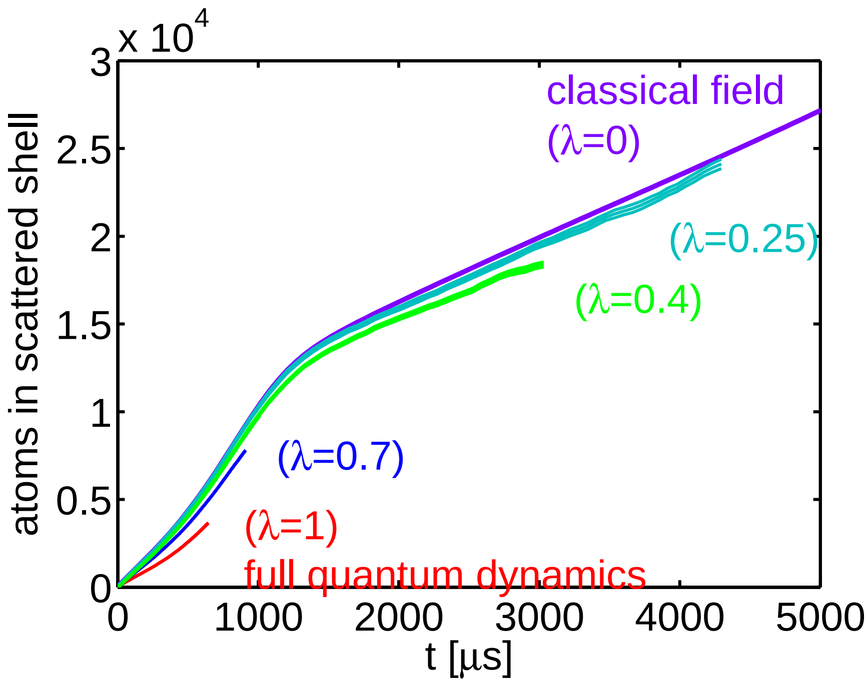
$$i\hbar\frac{d\widetilde{\psi}(x)}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + g\psi(x)\widetilde{\psi}^*(x) + f_2(\lambda)\sqrt{\frac{-g}{i\hbar}}\,\widetilde{\xi}(x,t)\right]\widetilde{\psi}(x)$$

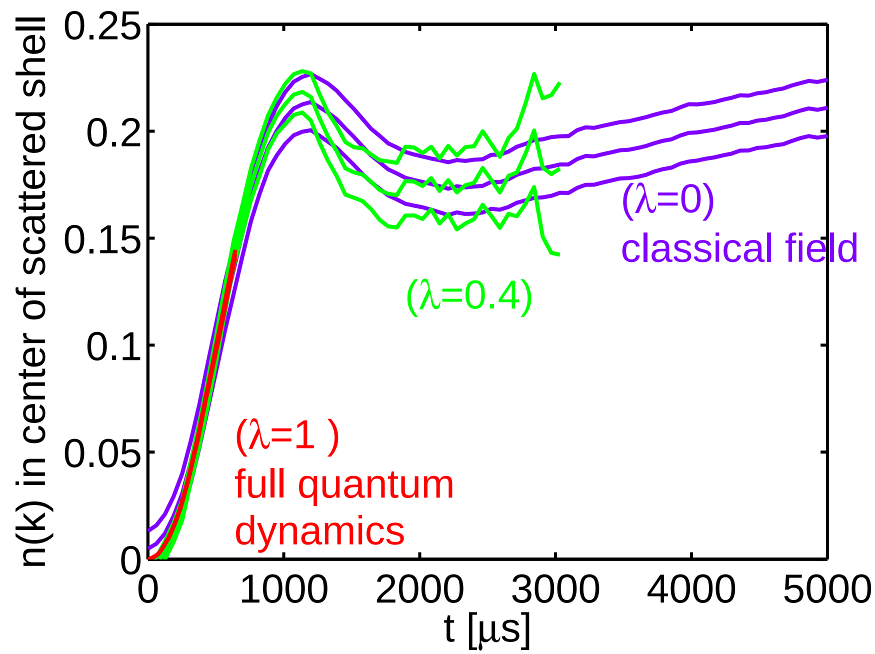
evolution

$$\overline{n}(x) = \left\langle\widehat{\Psi}^\dagger(x)\widehat{\Psi}(x)\right\rangle = \left\langle\widetilde{\psi}^*(x)\psi(x) - \frac{f_1(\lambda)}{2}\right\rangle_{\text{ensemble}}$$

observables

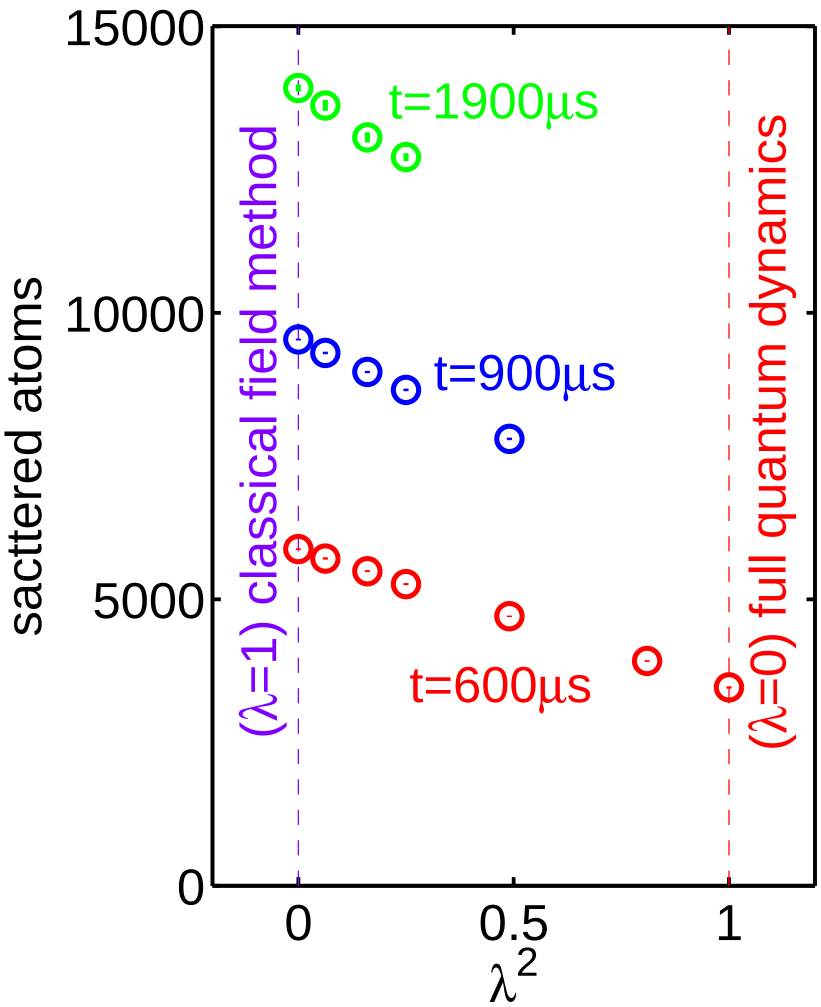
Resulting simulations





- Why combine bad features of both methods?
- Can get an idea of the size of the correction to the classical field method.
  e.g: total scattered number overestimated by several thousand
- Can verify some observables at long times
  e.g. density in main scattered shell is calculated correctly with classical field method

Estimating full quantum dynamics



- Calculate for various values of λ
- Here the observable varies linearly with λ^2
- Allows extrapolation to $\lambda = 1$ (full quantum dynamics) for much longer times

CONCLUSIONS:

- Quantitative assesment of classical field method accuracy
- Extrapolation to full QD for much longer times