

Photoassociation dynamics in a Bose-Einstein condensate

Thomas Gasenzer

Institut für Theoretische Physik

Universität Heidelberg

MESUMA04 DRESDEN

14 October 2004



Overview

- Microscopic Quantum Dynamics Approach
- Photoassociation — Rate limits
- Two-body dressed states
- Outlook

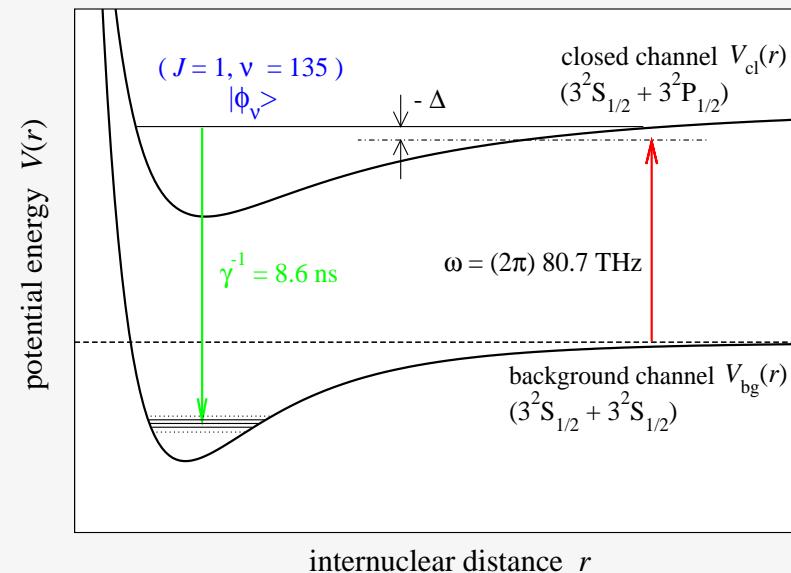
Funding:

Deutsche Forschungsgemeinschaft
A. v. Humboldt-Foundation

Introduction

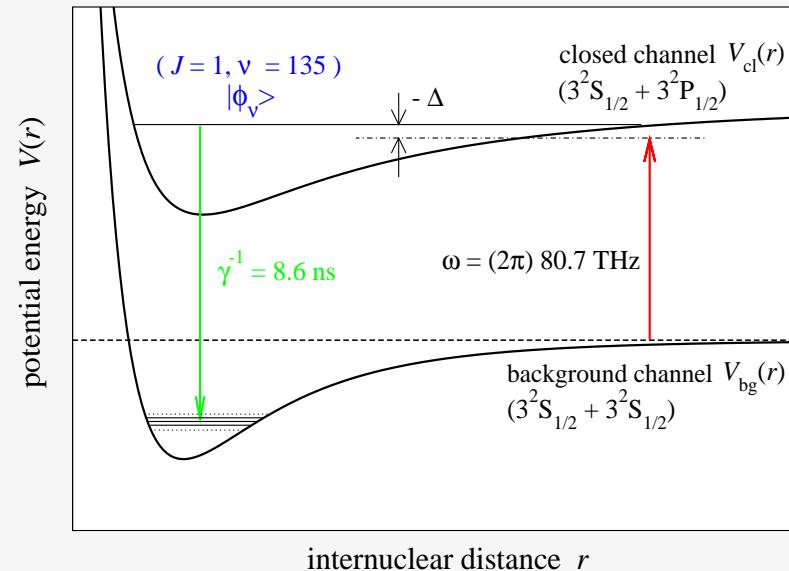
Single-colour photoassociation

Closed-channel bound state ϕ_v , coupled to
open channel by (detuned) laser light.



Single-colour photoassociation

Closed-channel bound state ϕ_ν , coupled to **open channel** by (detuned) laser light.

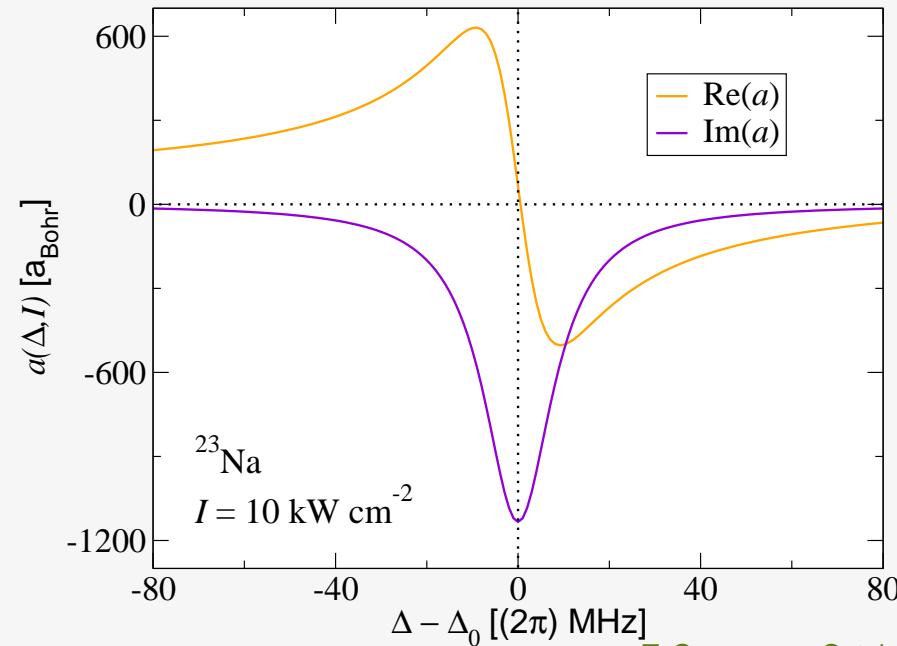


s-wave scattering length: $|a_0(\Delta, I)|$ remains finite if spontaneous electronic decay is present.

$$a(\Delta, I) = a_{bg} \left(1 - \frac{\Gamma(I)}{\Delta - \Delta_0(I) + \frac{i}{2}\gamma} \right)$$

P.O. Fedichev, Yu. Kagan, G.V. Shlyapnikov, J.T.M. Walraven,
PRL **77**, 2943 (1996)

J. Bohn, P.S. Julienne, PRA **54**, R4637 (1996)



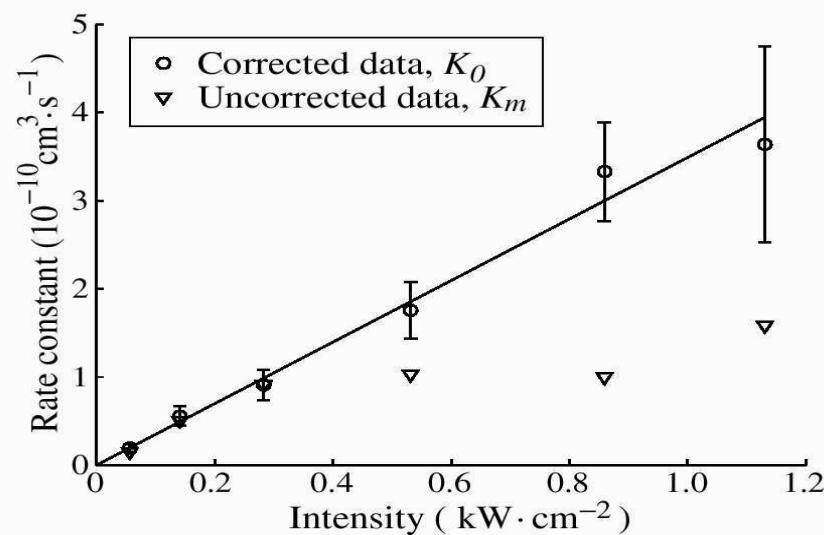
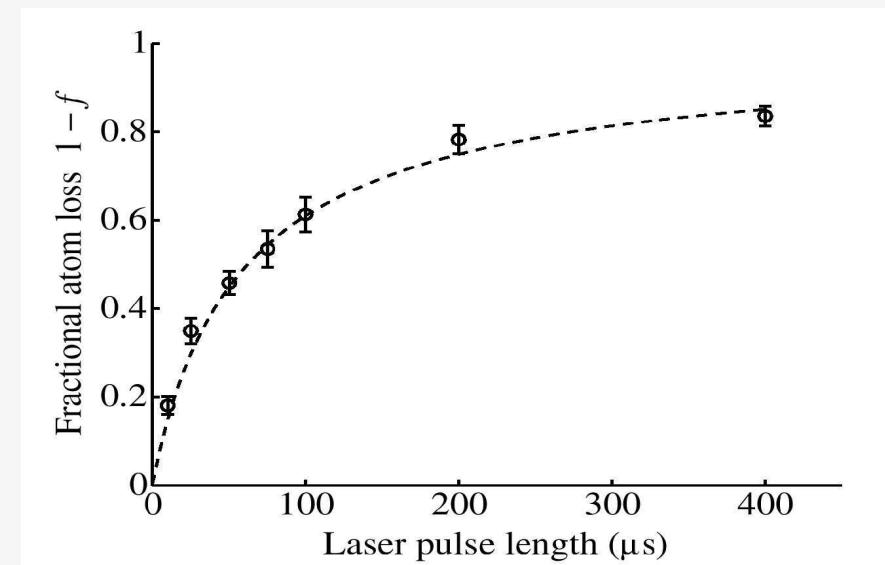
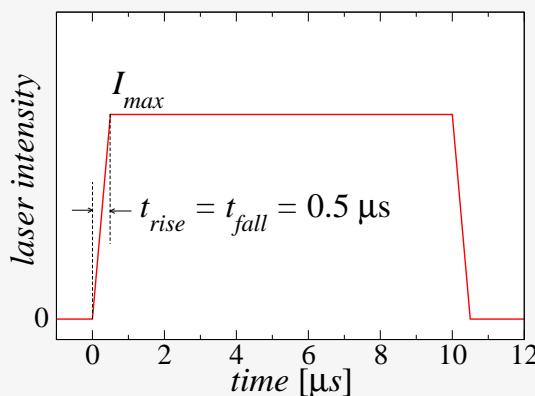
Experiment: Rate limits?

Single color PA of ^{23}Na (NIST).

[C. McKenzie, et al., PRL 88, 120403 (2002)]

GPE time evolution:

$$f = \frac{n(t, \mathbf{r})}{n(t_0, \mathbf{r})} = \frac{1}{1 + K_0(I)n(t_0, \mathbf{r})t}$$



Experimental and theoretical work

- **Experimental work** on rate limitation issues:

C. Drag, *et al.*, J. Quant. Electron. **36**, 1378 (2000).

C. McKenzie, *et al.*, PRL **88**, 120403 (2002).

U. Schlöder, C. Silber, T. Deusdle, and C. Zimmermann, PRA **66**, 061403 (2002).

I.D. Prodan, *et al.*, PRL **91**, 080402 (2003).

M. Weidemüller, R. Wester, *priv. comm.* (2004).

- Various **discussion** of rate limitations:

J.L. Bohn and P.S. Julienne, PRA **60**, 414 (1999).

K. Góral, M. Gaida, and K. Rzazewski, PRL **86**, 1397 (2001).

M. Holland, J. Park, and R. Walser, PRL **86**, 1915 (2001).

J. Javanainen and M. Mackie, PRL **88**, 090403 (2002).

Microscopic Quantum Dynamics Approach

Cumulant Approach

- **Dynamic equations** for correlation functions:

$$i\hbar \frac{\partial}{\partial t} \langle \psi(x) \rangle_t = \langle [\psi(x), H] \rangle_t$$

$$i\hbar \frac{\partial}{\partial t} \langle \psi(y)\psi(x) \rangle_t = \langle [\psi(y)\psi(x), H] \rangle_t$$

⋮

Cumulant Approach

- **Dynamic equations** for correlation functions:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \langle \psi(x) \rangle_t &= \langle [\psi(x), H] \rangle_t \\ i\hbar \frac{\partial}{\partial t} \langle \psi(y)\psi(x) \rangle_t &= \langle [\psi(y)\psi(x), H] \rangle_t \\ &\vdots \end{aligned}$$

- Resummation in terms of **cumulants (connected Green's functions)**:

$$\begin{aligned} \langle \psi(x) \rangle_t^c &= \langle \psi(x) \rangle_t \\ \langle \psi(y)\psi(x) \rangle_t^c &= \langle \psi(y)\psi(x) \rangle_t - \langle \psi(x) \rangle_t \langle \psi(y) \rangle_t \\ \langle \psi^\dagger(y)\psi(x) \rangle_t^c &= \langle \psi^\dagger(y)\psi(x) \rangle_t - \langle \psi^\dagger(x) \rangle_t \langle \psi(y) \rangle_t \\ &\vdots \end{aligned}$$

Cumulant Approach

- **Dynamic equations** for correlation functions:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \langle \psi(x) \rangle_t &= \langle [\psi(x), H] \rangle_t \\ i\hbar \frac{\partial}{\partial t} \langle \psi(y)\psi(x) \rangle_t &= \langle [\psi(y)\psi(x), H] \rangle_t \\ &\vdots \end{aligned}$$

- Resummation in terms of **cumulants (connected Green's functions)**:

$$\begin{aligned} \langle \psi(x) \rangle_t^c &= \langle \psi(x) \rangle_t \\ \langle \psi(y)\psi(x) \rangle_t^c &= \langle \psi(y)\psi(x) \rangle_t - \langle \psi(x) \rangle_t \langle \psi(y) \rangle_t \\ \langle \psi^\dagger(y)\psi(x) \rangle_t^c &= \langle \psi^\dagger(y)\psi(x) \rangle_t - \langle \psi^\dagger(x) \rangle_t \langle \psi(y) \rangle_t \\ &\vdots \end{aligned}$$

- Systematically truncate system of dynamic equations for the cumulants.

- ⇒ Few-body dynamics enters through ***T*-matrices**.
- ⇒ Energy & number conservation.
- ⇒ Positivity of mode occupations.

Mean Field Dynamics beyond Gross-Pitaevskii

- Dynamic equation for mean field $\Psi(\mathbf{x}, t) = \langle \psi(\mathbf{x}) \rangle_t^c$: $(\Phi = \langle \psi\psi \rangle_t^c)$

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{trap}}(\mathbf{x}) \right] \Psi(\mathbf{x}, t) + \int d^3y \, \mathbf{V}(\mathbf{x} - \mathbf{y}, t) \Psi^*(\mathbf{y}, t) \left[\Phi(\mathbf{x}, \mathbf{y}, t) + \Psi(\mathbf{x}, t) \Psi(\mathbf{y}, t) \right]$$

Mean Field Dynamics beyond Gross-Pitaevskii

- Dynamic equation for mean field $\Psi(\mathbf{x}, t) = \langle \psi(\mathbf{x}) \rangle_t^c$: $(\Phi = \langle \psi \psi \rangle_t^c)$

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{trap}}(\mathbf{x}) \right] \Psi(\mathbf{x}, t) + \int d^3y \, \mathbf{V}(\mathbf{x} - \mathbf{y}, t) \Psi^*(\mathbf{y}, t) \left[\Phi(\mathbf{x}, \mathbf{y}, t) + \Psi(\mathbf{x}, t) \Psi(\mathbf{y}, t) \right]$$

- **Non-Markovian** Nonlinear Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{trap}}(\mathbf{x}) \right] \Psi(\mathbf{x}, t) + \Psi^*(\mathbf{x}, t) \int_{t_0}^{\infty} d\tau \, g(t, \tau) \Psi^2(\mathbf{x}, \tau)$$

- Coupling function :

$$g(t, \tau) = (2\pi\hbar)^3 \langle 0 | \underbrace{\mathbf{V}(t)[\delta(t - \tau) + \mathbf{G}_{2B}(t, \tau)\mathbf{V}(\tau)]}_{T\text{-matrix!}} | 0 \rangle$$

Mean Field Dynamics beyond Gross-Pitaevskii

- Dynamic equation for mean field $\Psi(\mathbf{x}, t) = \langle \psi(\mathbf{x}) \rangle_t^c$: $(\Phi = \langle \psi \psi \rangle_t^c)$

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{trap}}(\mathbf{x}) \right] \Psi(\mathbf{x}, t) + \int d^3y \, \mathbf{V}(\mathbf{x} - \mathbf{y}, t) \Psi^*(\mathbf{y}, t) \left[\Phi(\mathbf{x}, \mathbf{y}, t) + \Psi(\mathbf{x}, t) \Psi(\mathbf{y}, t) \right]$$

- **Non-Markovian** Nonlinear Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{trap}}(\mathbf{x}) \right] \Psi(\mathbf{x}, t) + \Psi^*(\mathbf{x}, t) \int_{t_0}^{\infty} d\tau \, g(t, \tau) \Psi^2(\mathbf{x}, \tau)$$

- Coupling function :

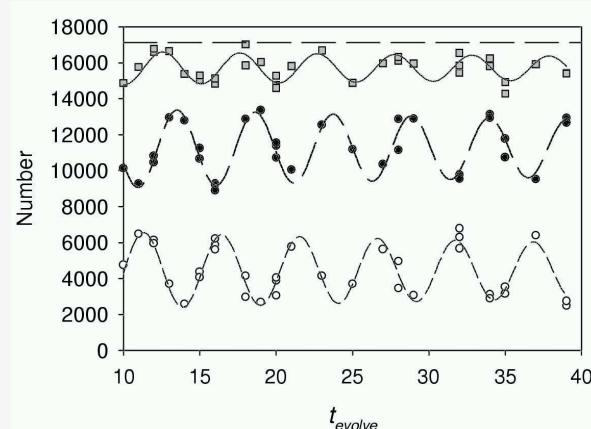
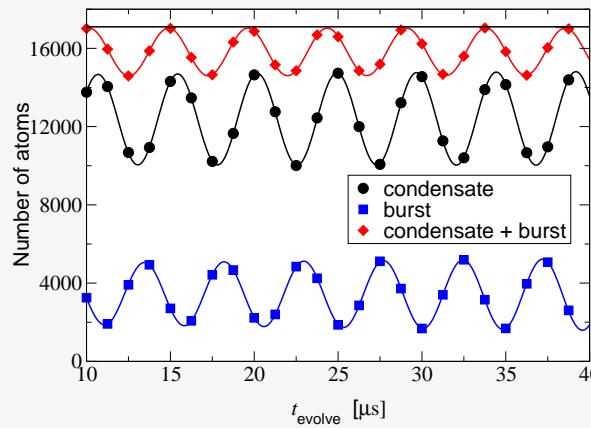
$$g(t, \tau) = (2\pi\hbar)^3 \langle 0 | \underbrace{\mathbf{V}(t)[\delta(t - \tau) + \mathbf{G}_{2B}(t, \tau)\mathbf{V}(\tau)]}_{T\text{-matrix!}} | 0 \rangle$$

- Markovian limit:
→ Gross-Pitaevskii dynamics:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{trap}}(\mathbf{x}) \right] \Psi(\mathbf{x}, t) + \frac{4\pi\hbar^2 a}{m} |\Psi(\mathbf{x}, t)|^2 \Psi(\mathbf{x}, t)$$

Previous applications of the Microscopic Quantum Dynamics Approach

Atom-molecule oscillations (JILA)

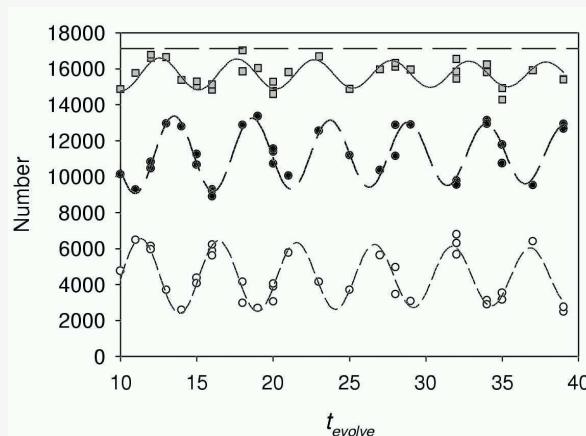
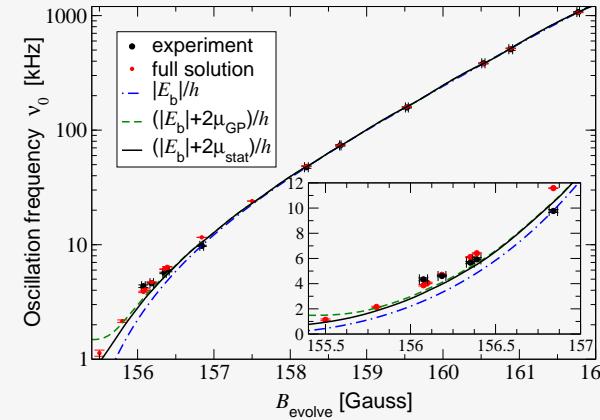
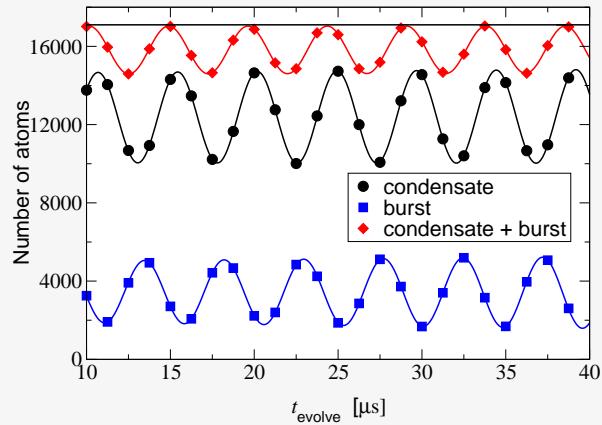


T. Köhler, T.G., and K. Burnett, PRA **67**, 13601 (03);

T. Köhler, T.G., P.S. Julienne, and K. Burnett, PRL **91**, 230401 (03).

Previous applications of the Microscopic Quantum Dynamics Approach

Atom-molecule oscillations (JILA)

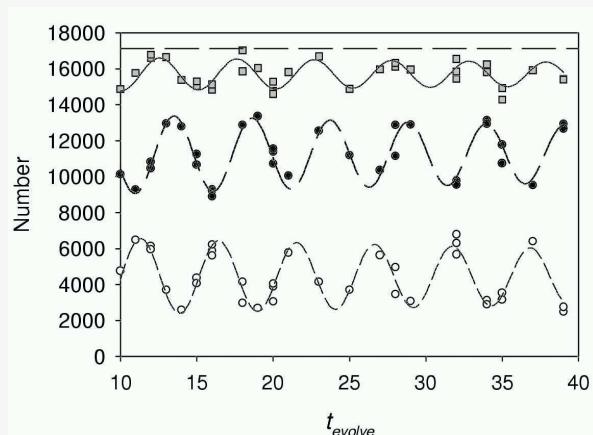
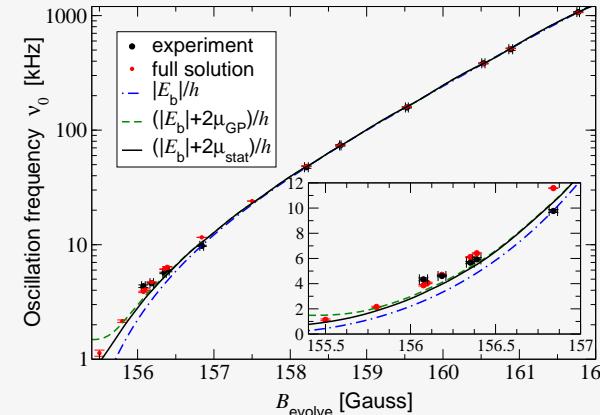
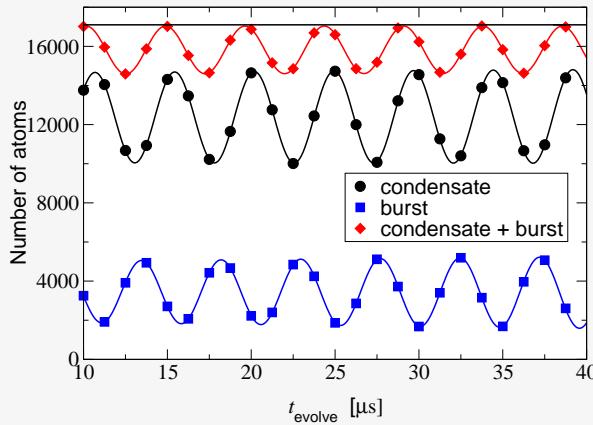


K. Góral, T. Köhler, and K. Burnett,
cond-mat/0407627.

T. Köhler, T.G., and K. Burnett, PRA **67**, 13601 (03);
T. Köhler, T.G., P.S. Julienne, and K. Burnett, PRL **91**, 230401 (03).

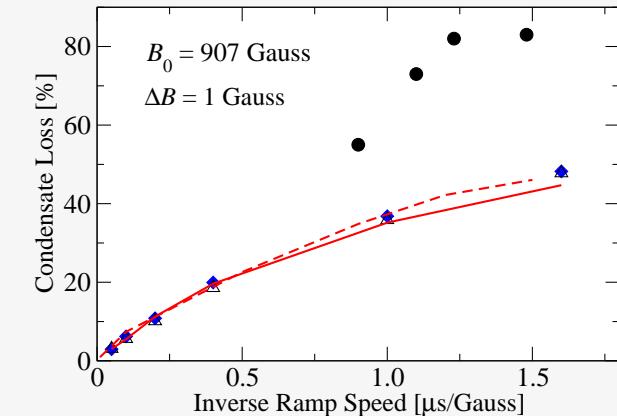
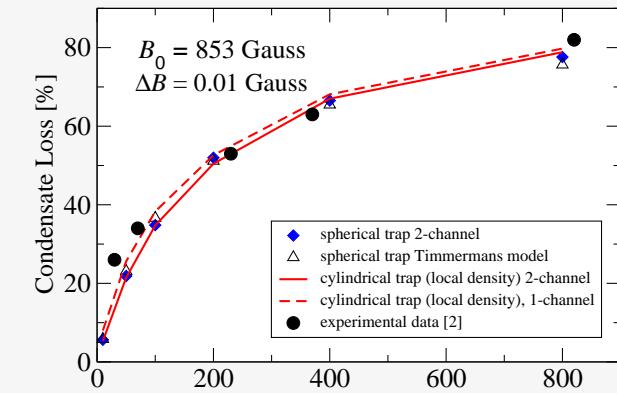
Previous applications of the Microscopic Quantum Dynamics Approach

Atom-molecule oscillations (JILA)



T. Köhler, T.G., and K. Burnett, PRA **67**, 13601 (03);
 T. Köhler, T.G., P.S. Julienne, and K. Burnett, PRL **91**, 230401 (03).

Feshbach ramps, e.g., @ MIT

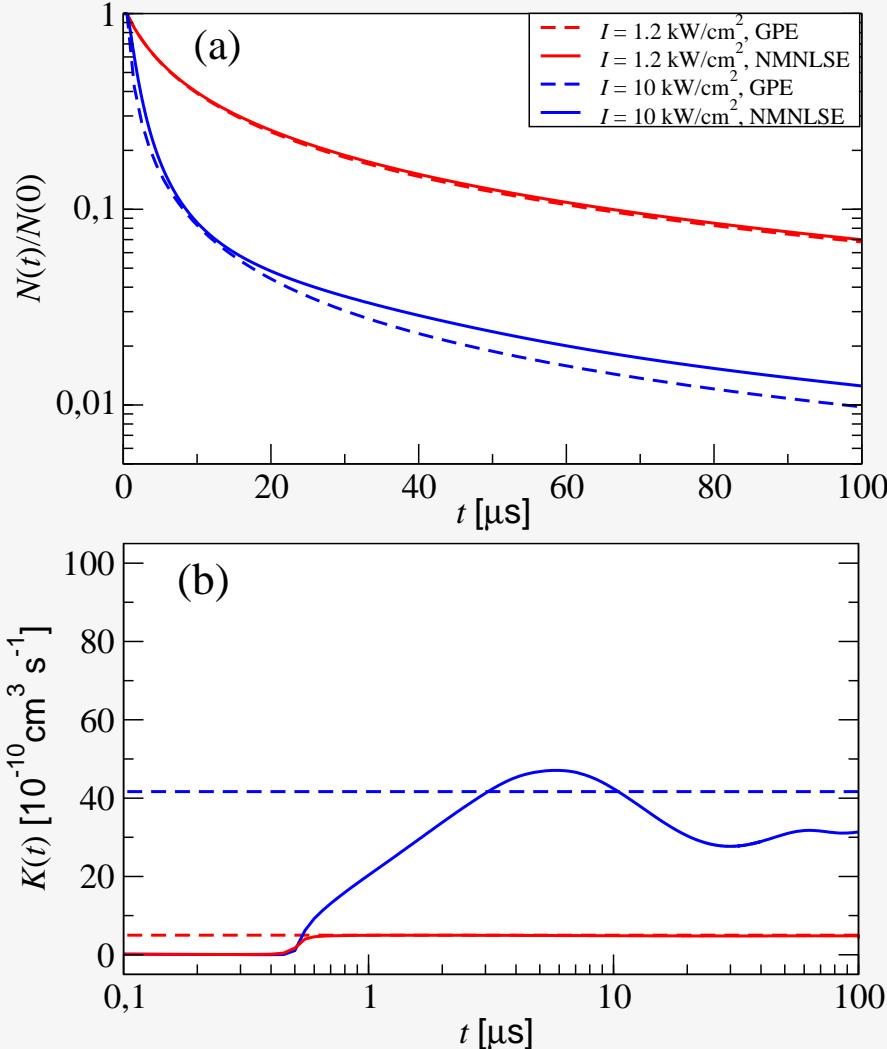


T. Köhler, K. Goral, and T.G., PRA **70**, 23613 (04).

Photoassociation

Rate limits

Photoassociation in ^{23}Na condensate: Is the loss rate limited?



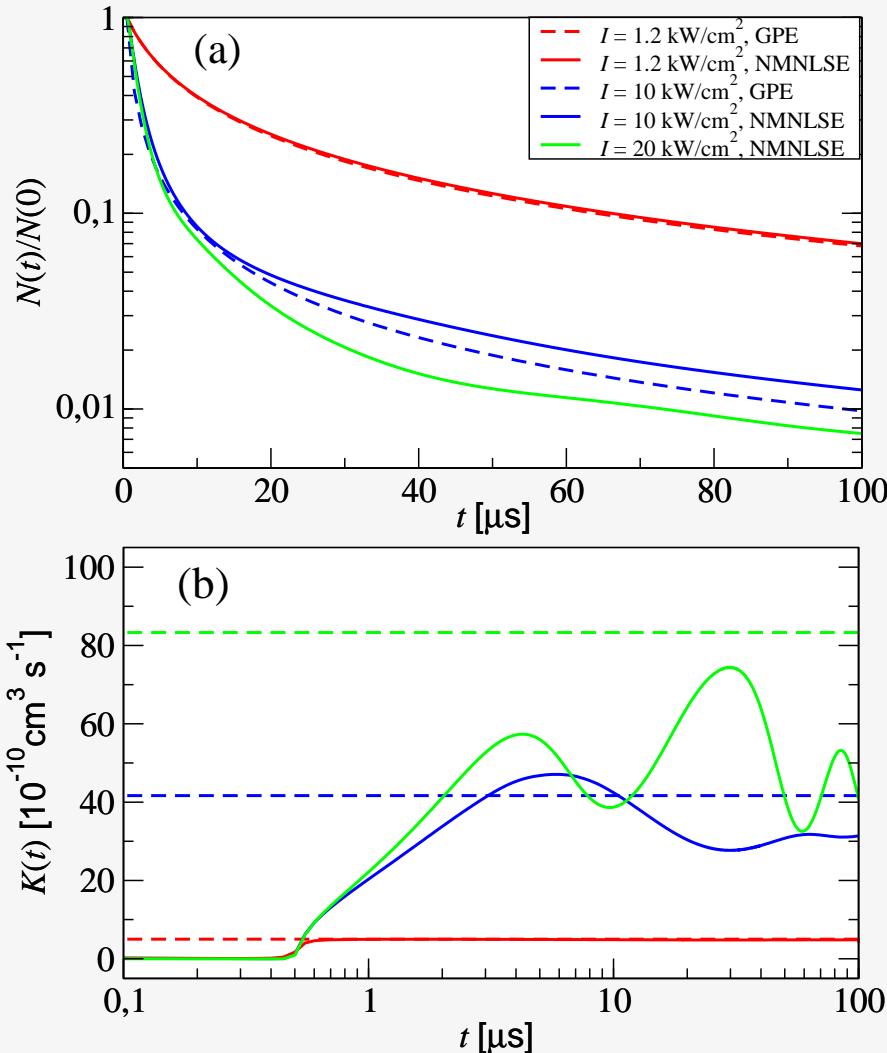
Evolution of the **remaining fraction** of $N(0) = 4.0 \cdot 10^6$ condensate atoms in spherical harmonic ($\nu = 198 \text{ Hz}$) trap, for laser intensity I .

GPE time evolution:

$$n(t, r) = \frac{n(t_0, r)}{1 + K(I)n(t_0, r)t}$$

Temporally local decay ‘rate’:
 $K(t) = -\dot{N}(t) / \int dx n(x, t)^2$

Photoassociation in ^{23}Na condensate: Is the loss rate limited?



Evolution of the **remaining fraction** of $N(0) = 4.0 \cdot 10^6$ condensate atoms in spherical harmonic ($\nu = 198 \text{ Hz}$) trap, for laser intensity I .

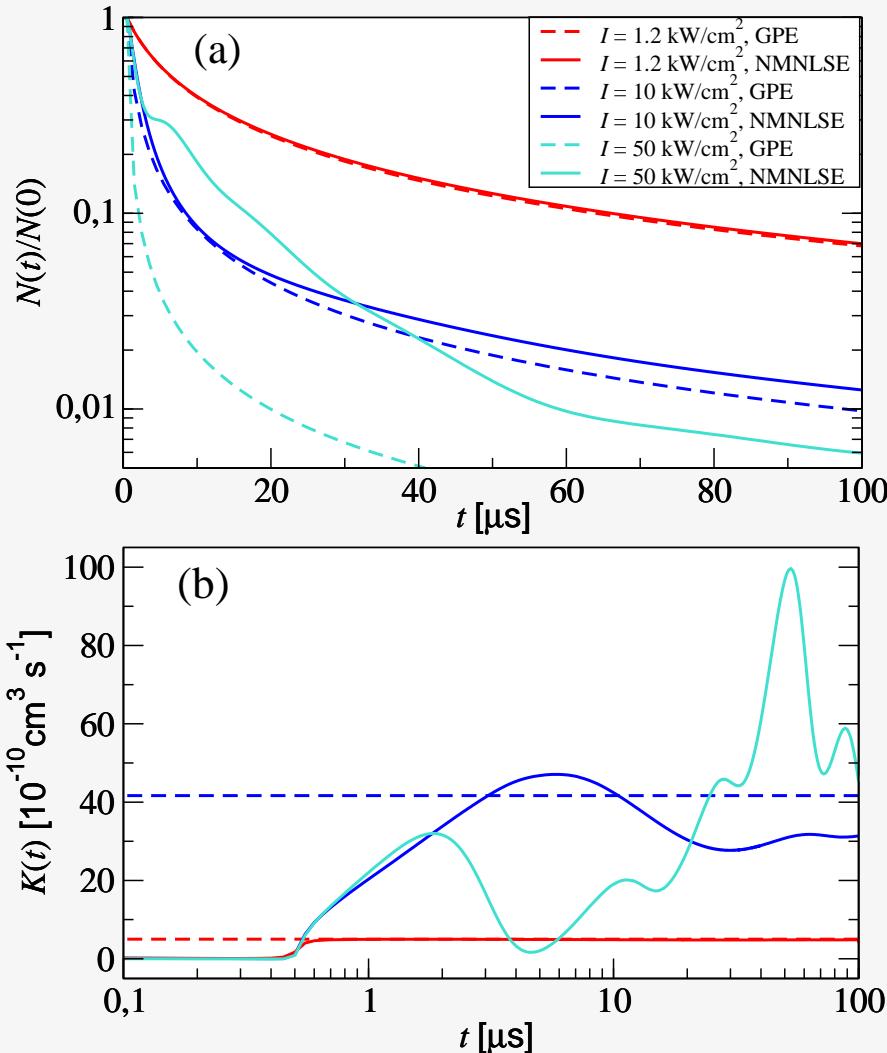
GPE time evolution:

$$n(t, r) = \frac{n(t_0, r)}{1 + K(I)n(t_0, r)t}$$

Temporally local decay ‘rate’:
 $K(t) = -\dot{N}(t) / \int dx n(x, t)^2$

[T.G., PRA **70**, 021603(R) (2004); cond-mat/0406629 (PRA, in press)]

Photoassociation in ^{23}Na condensate: Is the loss rate limited?



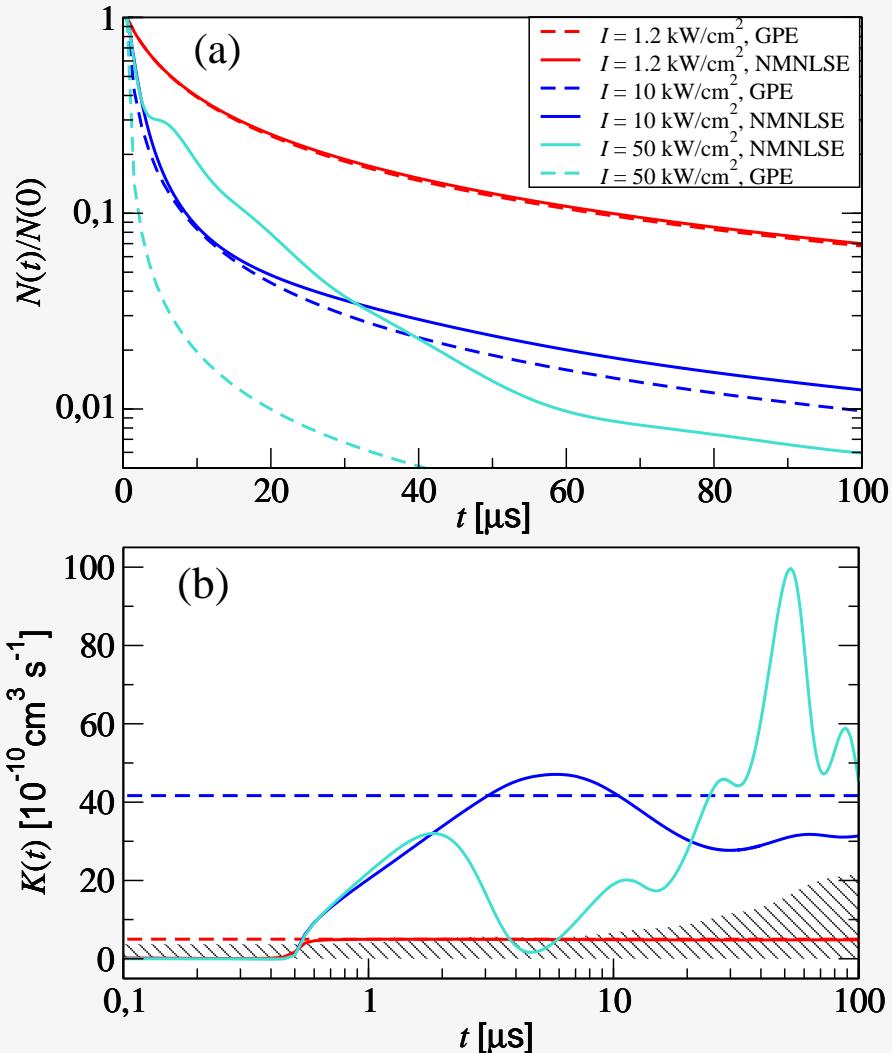
Evolution of the **remaining fraction** of $N(0) = 4.0 \cdot 10^6$ condensate atoms in spherical harmonic ($\nu = 198 \text{ Hz}$) trap, for laser intensity I .

GPE time evolution:

$$n(t, r) = \frac{n(t_0, r)}{1 + K(I)n(t_0, r)t}$$

Temporally local decay ‘rate’:
 $K(t) = -\dot{N}(t) / \int dx n(x, t)^2$

Photoassociation in ^{23}Na condensate: Is the loss rate limited?



Evolution of the **remaining fraction** of $N(0) = 4.0 \cdot 10^6$ condensate atoms in spherical harmonic ($\nu = 198$ Hz) trap, for laser intensity I .

GPE time evolution:

$$n(t, r) = \frac{n(t_0, r)}{1 + K(I)n(t_0, r)t}$$

Temporally local decay ‘rate’:

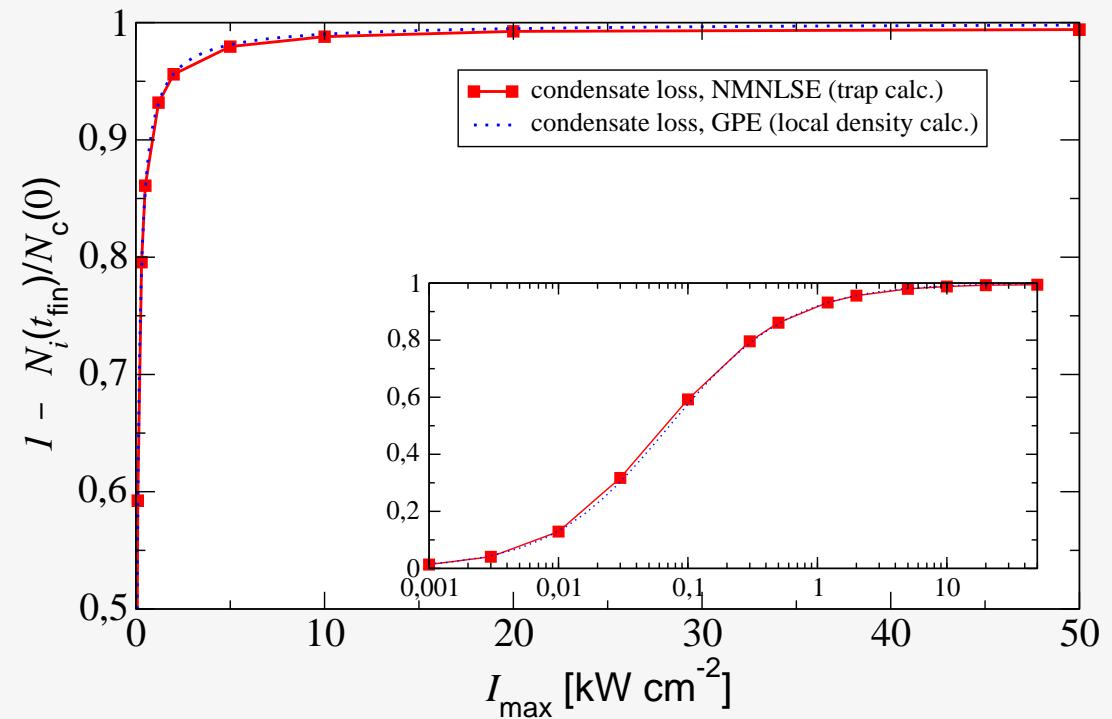
$$K(t) = -\dot{N}(t) / \int dx n(x, t)^2$$

Max. local decay rate according to

$$K_J(R, t) = (\hbar/m)[n_c(R, t)]^{-1/3} \quad (\text{hatched})$$

Photoassociation in ^{23}Na condensate: Is the molecule formation rate limited?

Fraction of condensate atoms lost after
 $t = 100 \mu\text{s}$ (red squares).

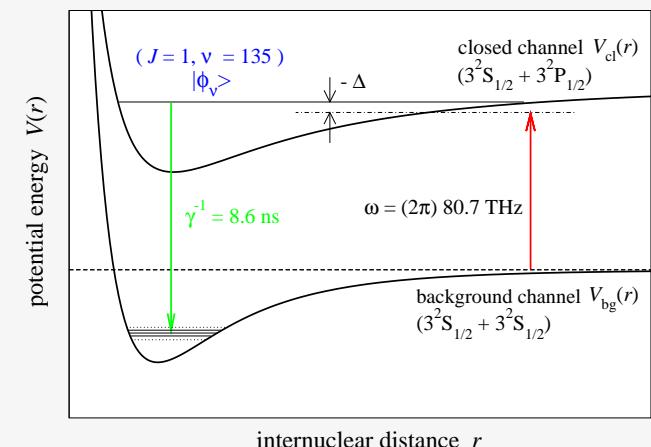
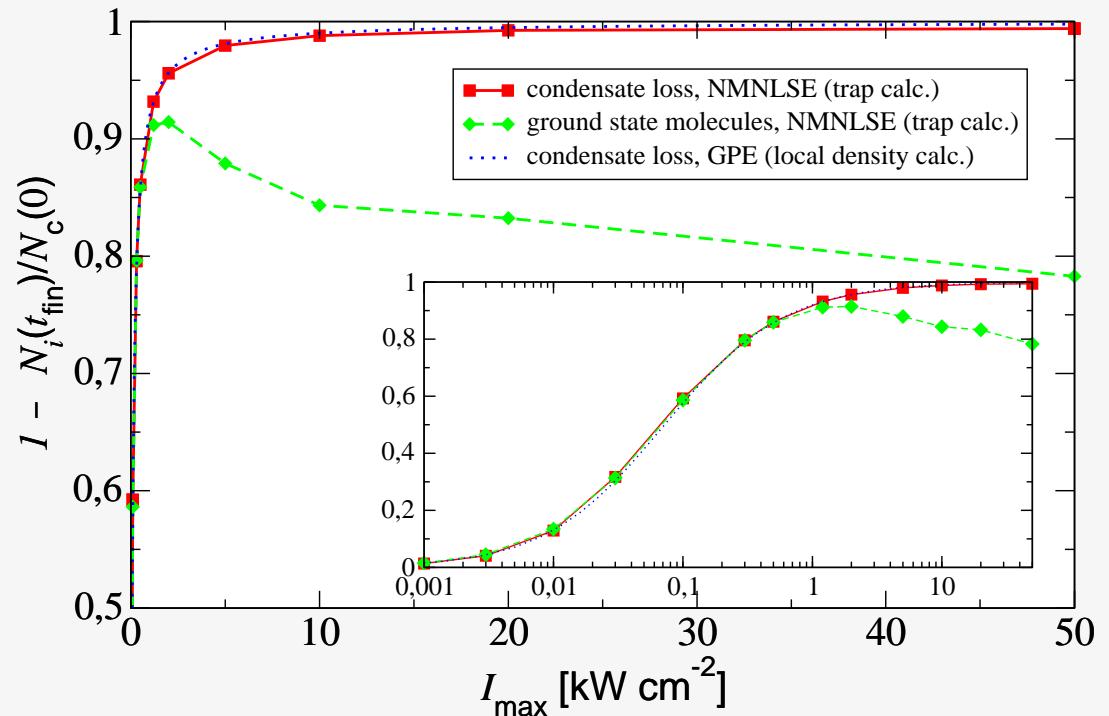


Photoassociation in ^{23}Na condensate: Is the molecule formation rate limited?

Fraction of condensate atoms lost after
 $t = 100 \mu\text{s}$ (red squares).

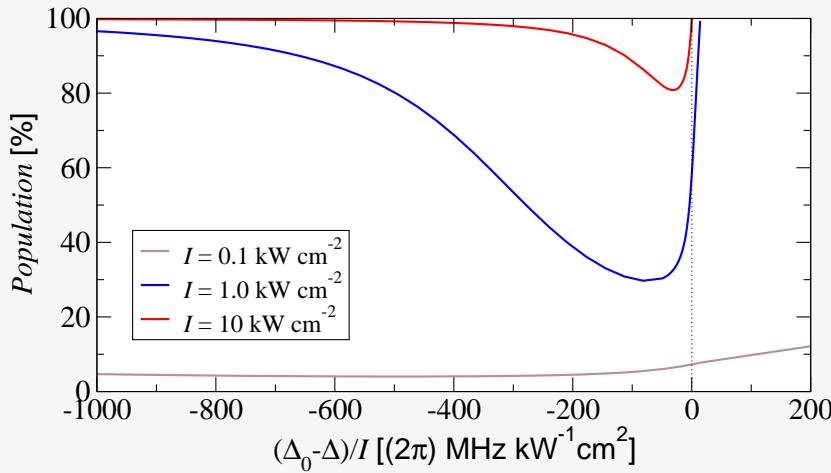
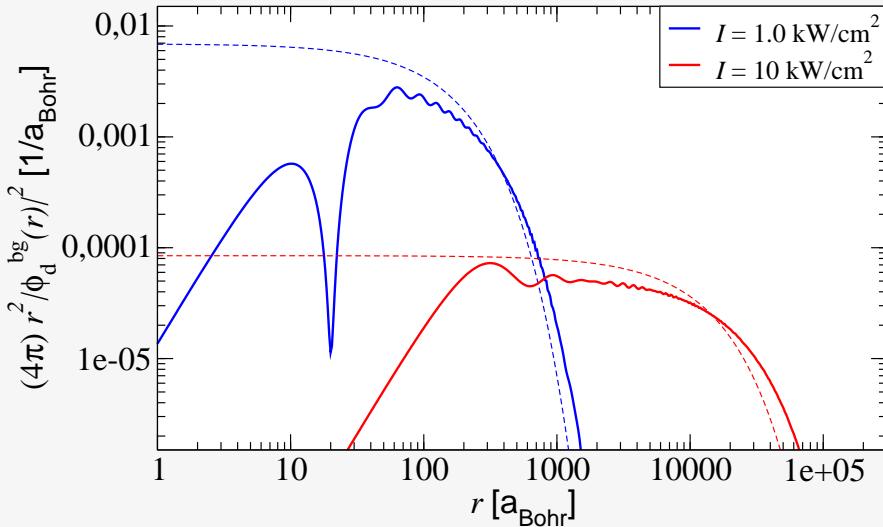
Compare this fraction to the fraction of
the number of atoms lost via spontaneous
decay (green diamonds):

$$\hbar \dot{N}_{\text{tot}} = -\gamma \int d\mathbf{R} \left| \int d\mathbf{r} \tilde{\phi}_\nu^*(\mathbf{r}) \Phi_{\text{cl}}(\mathbf{R}, \mathbf{r}, t) \right|^2.$$



Two-body dressed states

Saturation of loss rates due to Long range nature of dressed states



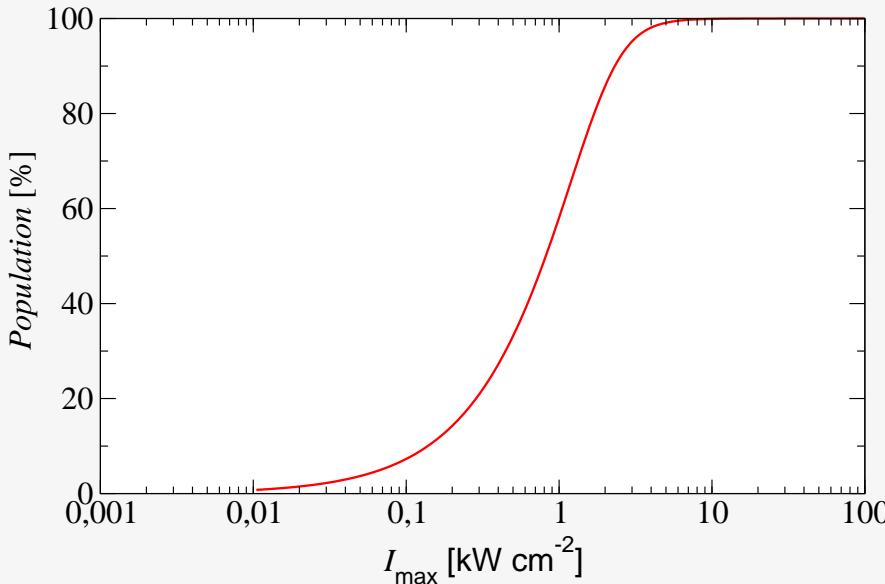
Background channel component of radial
dressed state density.

$$\Delta - \Delta_0(I) = 0.$$
$$\phi_d^{bg}(r) \simeq \frac{e^{-r/\alpha(\Delta, I)}}{r} \quad (\text{---})$$

Population
of background channel component:

$$(\mathcal{N}_d^2 - 1)/\mathcal{N}_d^2$$

Population of Background channel dressed state component

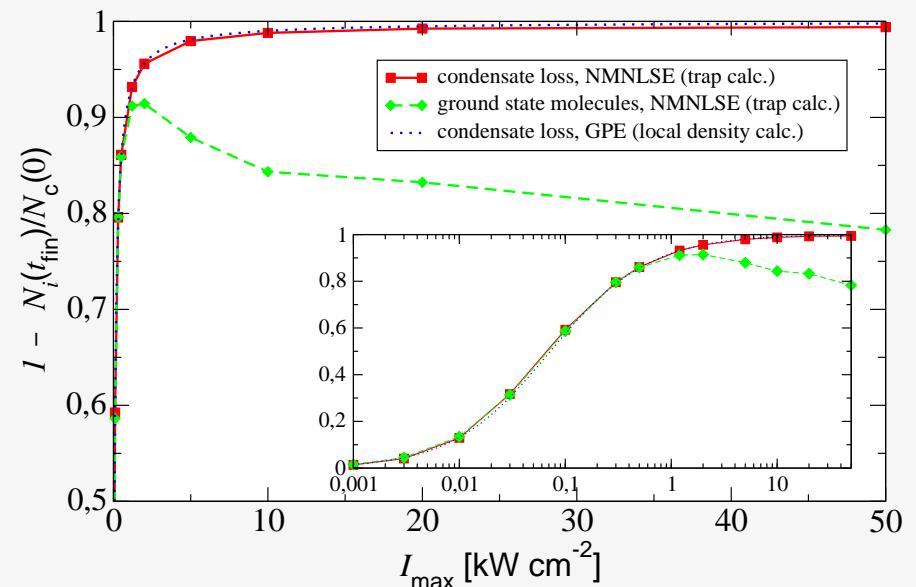


Compare this to the fraction of the number of atoms lost via spontaneous decay (green diamonds):

$$\hbar \dot{N}_{\text{tot}} = -\gamma \int d\mathbf{R} \left| \int dr \tilde{\phi}_{\nu}^*(\mathbf{r}) \Phi_{\text{cl}}(\mathbf{R}, \mathbf{r}, t) \right|^2.$$

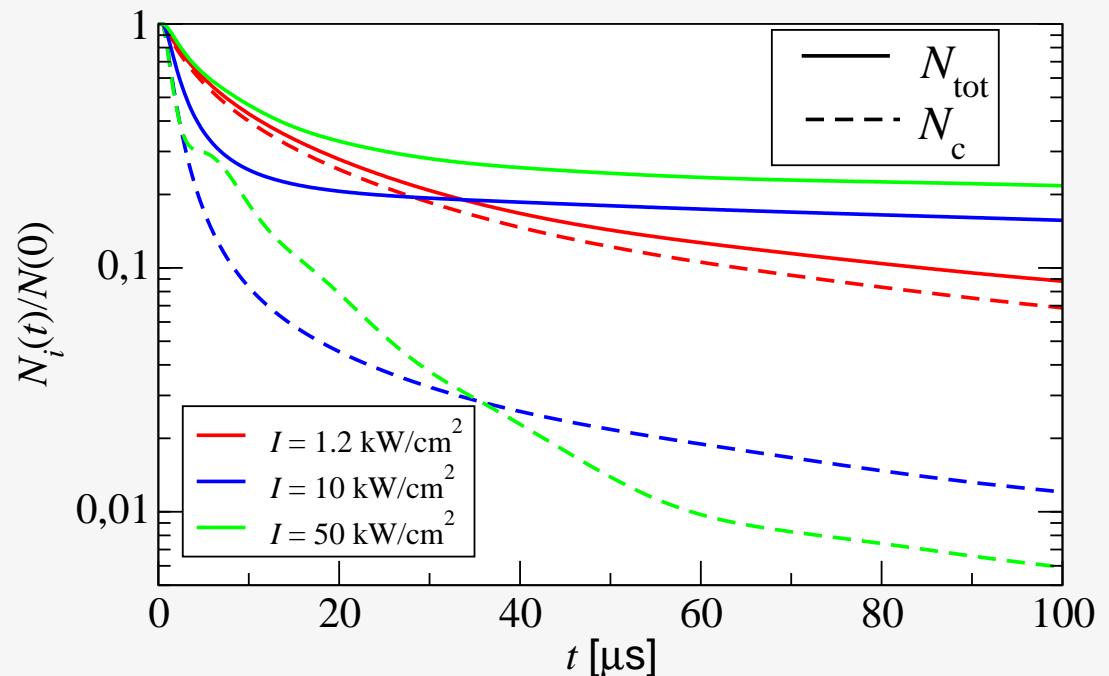
Population $(\mathcal{N}_d^2 - 1)/\mathcal{N}_d^2$ of **background channel component** vs. intensity I (on resonance, $\Delta = \Delta_0(I)$).

$$\begin{pmatrix} \phi_d^{\text{bg}} \\ \phi_d^{\text{cl}} \end{pmatrix} = \mathcal{N}_d^{-1} \begin{pmatrix} G_{\text{bg}}(E_d) W \phi_{\nu} \\ \phi_{\nu} \end{pmatrix}$$



Photoassociation in ^{23}Na condensate: Is the molecule formation rate limited?

Fractions of condensate (---) and total (—) atom no. loss, as a function of time, for different intensities.



Open Questions Outlook

- Photoassociation:
 - heteronuclear PA, STIRAP, ...
 - Alkaline earth elements: small decay width γ , large scattering lengths

(→ metrology)

- non-universal observables (many-body frequency shifts)

- Fermionic and mixed systems:

- Molecular BEC
- BCS pairing

- Improved truncation schemes on the basis of the 2PI effective action

$$\Gamma[\Psi, \textcolor{blue}{G}] = S[\Psi] + \frac{i}{2} \text{Tr} \ln(\textcolor{blue}{G}^{-1} + G_0^{-1}(\Psi) \textcolor{blue}{G}) + \Gamma_2[\Psi, \textcolor{blue}{G}]$$

[G. Aarts, *et al.*, PRD **66**, 045008 (2002)]

- Condensates in microtraps: far-from-equilibrium dynamics in (quasi) one-dimensional regime

- Long-time evolution (damping, drifting, thermalization)