Hot topics in cold atom theory

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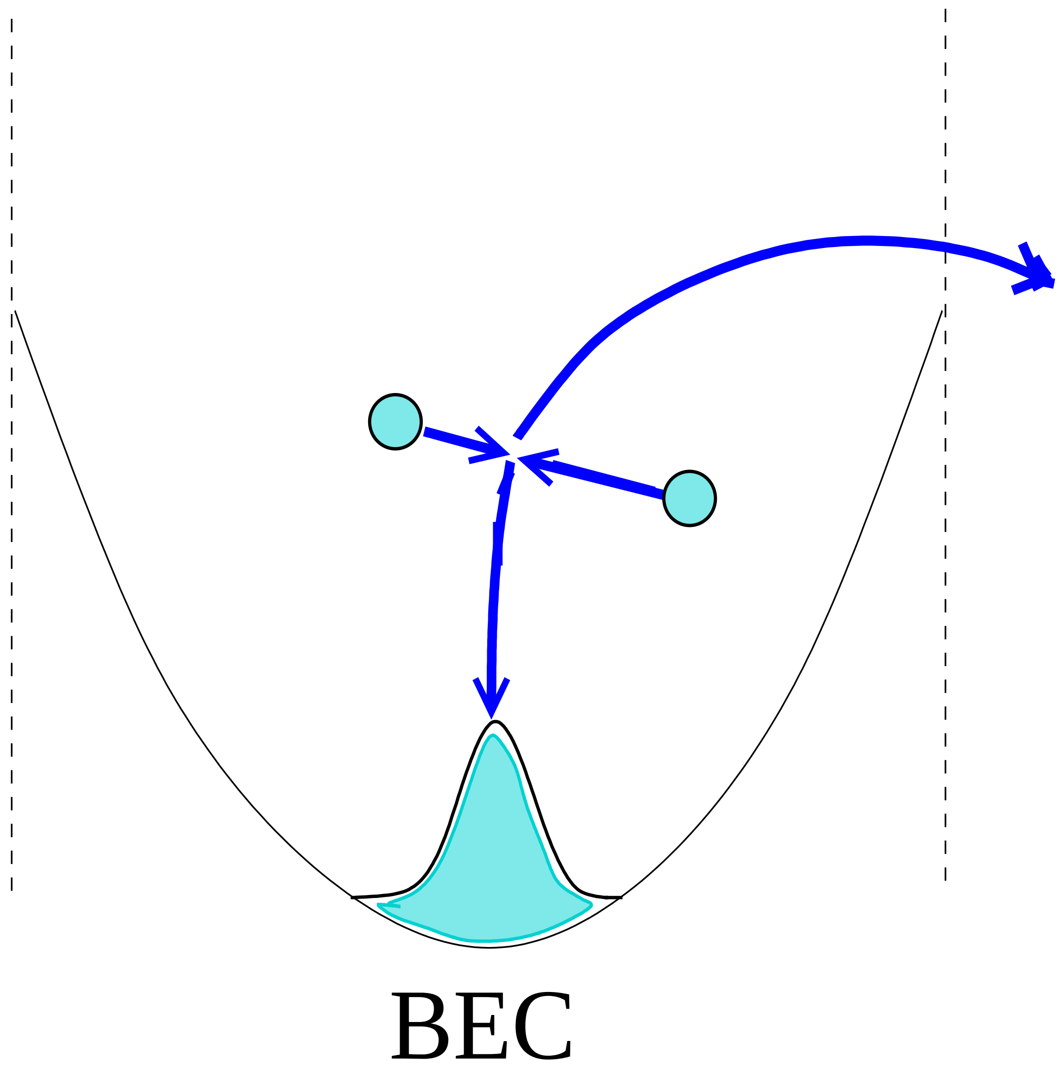
Burning questions in nano-Kelvin physics!

- **Quantum evaporative cooling** - what is the *quantum* state of a BEC?
- **Bose-Einstein nucleation** - is a growing BEC ever *hot*?
- **Mode-locking atom lasers** - when are atomic pulse-trains *coherent*?
- **Superchemistry** - how do atom *waves* interact to make molecules?
- **Classical solitons** - can BEC matter become *stable* in free space?
- **Quantum singularities** - are there *localised* quantum states in a 3D BEC?

Quantum evaporative cooling

- What is the true state of a *real* BEC?



- Collisions of hot atoms lead to condensate formation

Dynamical problem!

- Initially a hot multimode system; interacting particles in a finite trap
- Quantum fluctuations important near critical point
- What state does the evaporation process lead to?
- Is it really in thermal equilibrium?
- Use quantum phase-space methods (quasi-probabilities)
- Retains quantum features; allows multimode simulation

Quantum dynamics

- "Can a quantum system be probabilistically simulated by a classical universal computer? ...If you take the computer to be the classical kind I've described so far, ... the answer is certainly, No!" (Richard P. Feynman *Simulating Physics with Computers*)

- "Hence the implications of Feynman's argument seems to be that we really cannot simulate quantum dynamics on a local classical computer....... " (David M. Ceperley, *The Simulation of Quantum Systems*)

- "The equivalent to Molecular Dynamics (Quantum Molecular Dynamics) does not exist in any practical sense... One is forced to either simulate very small systems (i.e. less than five particles) or to make serious approximations." (David M. Ceperley, *Lectures on Quantum Monte Carlo*, May 1996)

- **We simulate $10,000$ atoms in 32000 trap modes; 10^{10000} states in Hilbert space.**

+P representation

- expand quantum density matrix $\hat{\rho}$ in off-diagonal coherent state projection operators:

$$\hat{\rho} = \int P(\psi_1, \psi_2) \frac{|\psi_1\rangle\langle\psi_2|}{\langle\psi_2|\psi_1\rangle} \mathcal{D}\psi_1 \mathcal{D}\psi_2$$

- $\mathcal{D}\psi_1$, $\mathcal{D}\psi_2$ are the functional measures over coherent states

- $P(\psi_1, \psi_2)$ is a positive distribution function which exists for all density matrices

- when the boundary terms in the integration vanish, P is governed by a Fokker-Planck equation (FPE)

- the FPE leads to two stochastic phase-space equations

- used to successfully predict quantum soliton behaviour in optical fibers [NATURE 365, pp307]

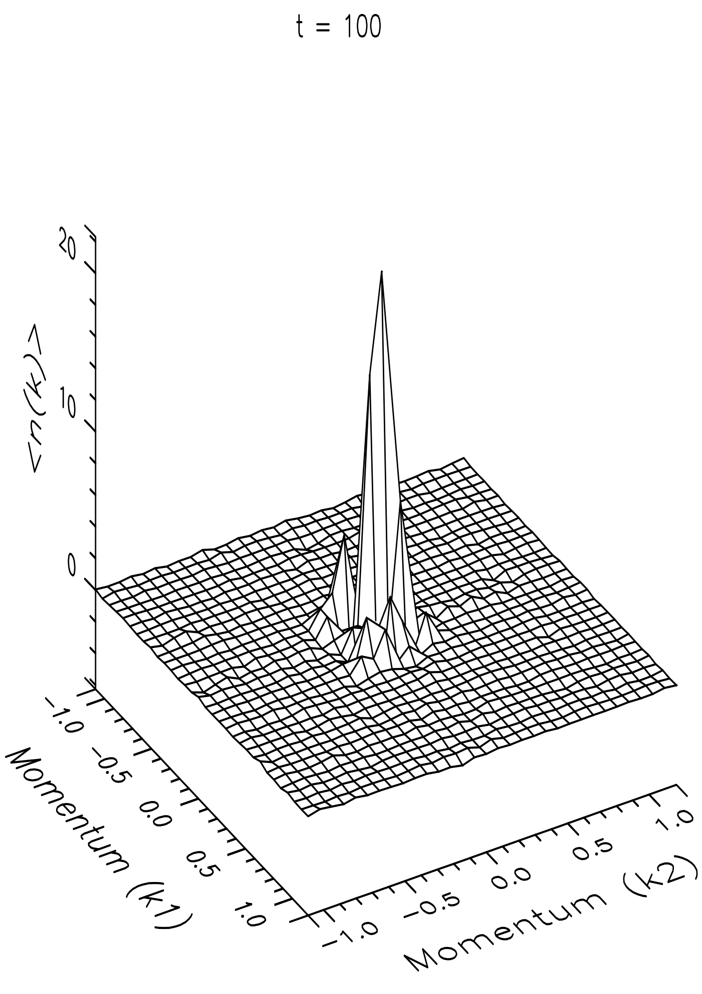
+P Stochastic Equations

$$i\hbar\frac{\partial\psi_j}{\partial t} = [\frac{-\hbar^2\nabla^2}{2m} + V - \frac{i\hbar}{2}\Gamma + U\psi_j\psi^*_{3-j} + \sqrt{i\hbar U}\xi_j]\psi_j$$

- $j = 1, 2$; $m =$ atomic mass
- $V(\mathbf{x}) =$ trapping potential
- $\Gamma(\mathbf{x}) =$ loss rate
- $U =$ atom-atom coupling
- $\langle\xi_i(t,\mathbf{x})\xi_j(t',\mathbf{x}') = \delta_{ij}\delta(t-t')\delta(\mathbf{x}-\mathbf{x}')$ - stochastic term
- $\psi_2^*\psi_1 = \hat{\Psi}_2^{+}\hat{\Psi}_1 =$atom density

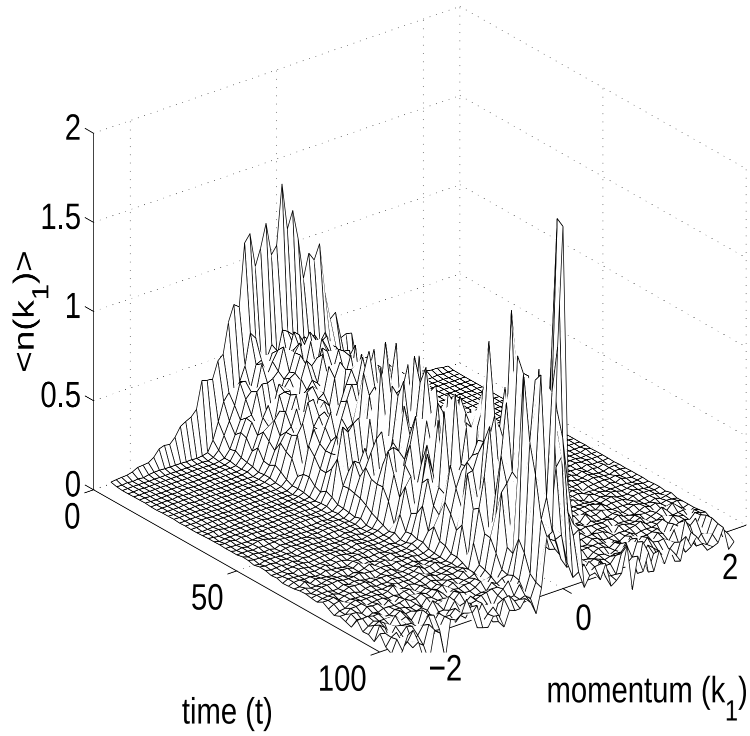
3D Bose condensation: one trajectory

2D cross-section of density in momentum space after evaporative cooling; large occupation numbers.



3D Bose Condensation: Ensemble average

Phase-space densities are reduced on average due to the random condensation into low-lying excited states of the center-of-mass motion!



SUMMARY

- first principles quantum simulation of BEC. [Drummond & Corney, PRA 60, R2661 (1999)].
- results limited by the stochastic sampling error (needs improved basis set)
- extremely difficult - not impossible with classical computers
- physics: evaporative cooling with variable potential
- condensate typically forms in excited mode, with metastable vortices
- **Condensates have spontaneous center-of-mass motion.**

II: Bose-Einstein nucleation -

- how can a growing BEC get *hot*?

- The essential feature of our model of a one-component trapped Bose condensate, is the D dimensional Gross-Pitaevskii (GP) equation with a linear gain term g, of the form:

$$i\frac{\partial\Psi(t,\mathbf{x})}{\partial t} = \left[ig + \frac{-\hbar}{2m}\nabla^2_{\mathbf{x}} + \frac{V(x)}{\hbar} + \kappa|\Psi|^2\right]\Psi(t,\mathbf{x})\,.$$

- Here the potential term V is due to an optical or magnetic trap:

$$V(\mathbf{x}) = \sum m|x_i|^2\omega_i^2/2$$

.

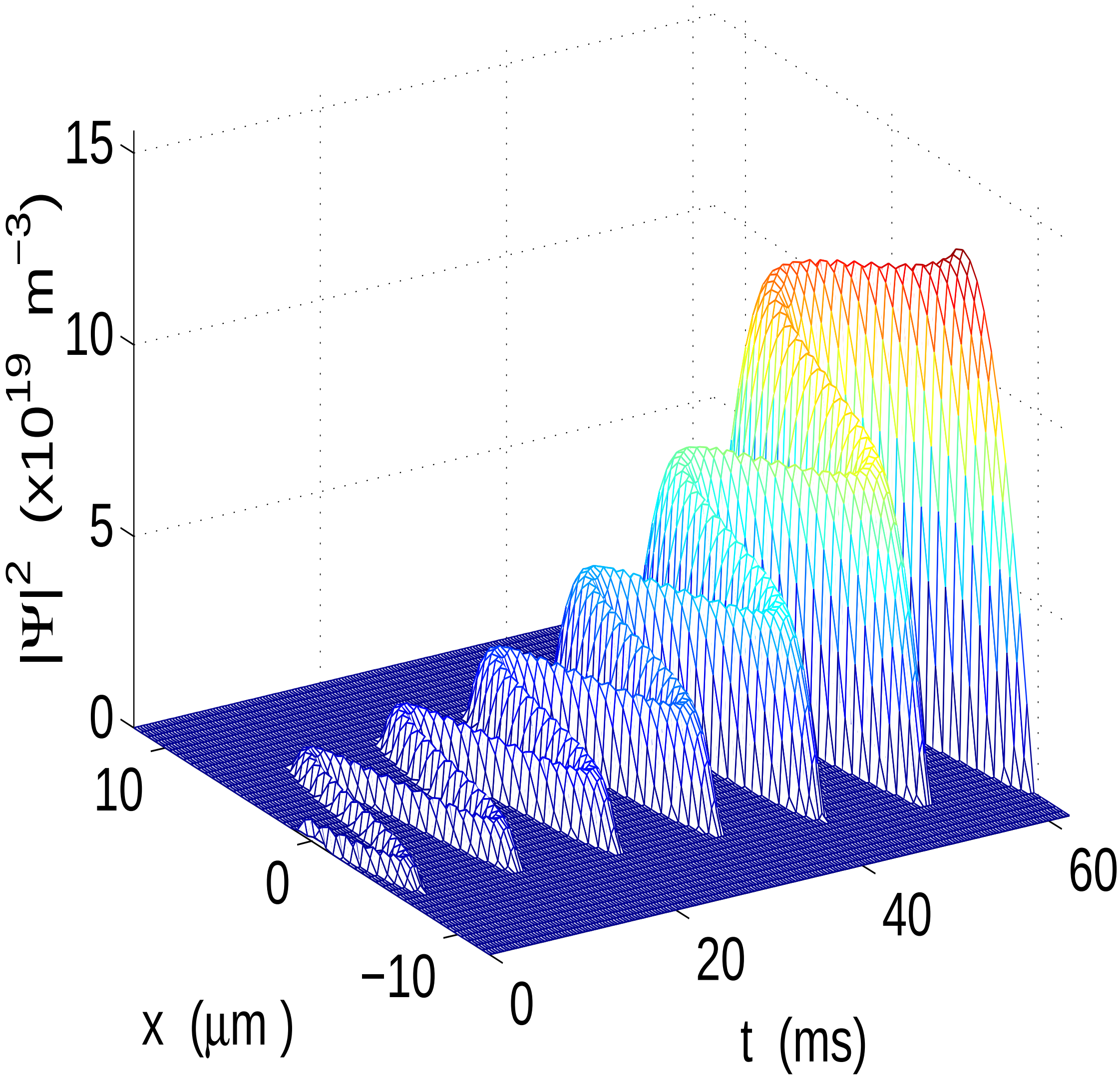
-Solution:

The asymptotic solution (at large growth time, but before saturation):

$$|\Psi(t,\mathbf{x})|^2 = \rho_0 e^{2\tilde{g}t}\left(1 - \frac{|\mathbf{x}-\mathbf{x}_0(t)|^2}{R(t)^2}\right)$$

- $\tilde{g} = 2g/(2+D)$
- $R(t) = R_0 e^{\tilde{g}t}/\sqrt{\tilde{g}^2+\omega^2}$
- $\mathbf{x}_0(t) = \sum \mathbf{a}_i cos(\omega_i t + \delta_i)$

Graph of analytic solution



SUMMARY

- The C.O.M. kinetic energy INCREASES with time, since the amplitude is unchanged with time:

$$E_{COM} = N_0 e^{2gt} \times \frac{1}{2} \sum m |\mathbf{a}_i|^2 \omega_i^2$$

- Hence a BEC has a cold relative temperature, but the COM energy is not cooled by evaporation!

- Quadratic density pulses also observed in optical fibers (Harvey et al, PRL, to appear 2000)

- Effects like this are often observed experimentally.

- Usually attributed to trap technical noise.

- **This is a non-equilibrium system, with multiple temperatures!**

III: Mode-locking atom lasers

- When are atomic pulse-trains *coherent*?
- We suggest making use of atom-atom repulsion, to form a stable dark soliton in a toroidal trap.
- A periodic output coupler is added using a Raman laser.
- This forms a modelocked, pulsed atom laser.
- **The atom laser output pulses are in all phase with each other.**

Toroidal trap equations

In the limit of a deep trap, we suppose that any mode-structure transverse to the trap circumference can be neglected. This gives a dimensionless G-P equation on the torus, where α is the nonlinearity:

$$i\frac{\partial\psi}{\partial\tau} = -\frac{\partial^2\psi}{\partial\theta^2} + \alpha|\psi|^2\psi\,.$$

The normalization and periodicity conditions are :

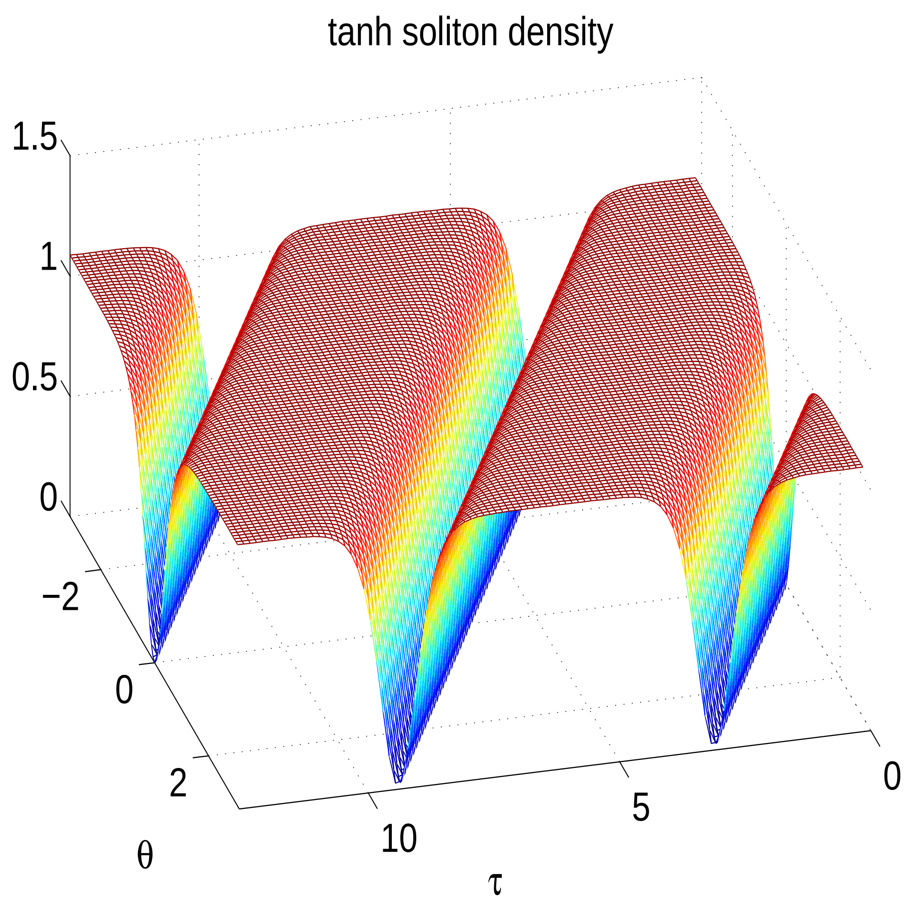
$$\int_0^{2\pi} d\theta\psi^*\psi = 2\pi\,,$$

$$\psi(\theta + 2\pi, \tau) = \psi(\theta, \tau)\,.$$

Tanh with a twist

For large α, we find the solution **with** $l = 1/2$:

$$\psi(\bar{\theta}) \simeq \tanh\left(\sqrt{\frac{\alpha}{2}}\,(\bar{\theta} - \pi/s)\right) e^{i(\bar{\theta}/2 - \omega\tau)} . \quad (1)$$



Mode-locked atom laser

We now include a stirring potential, gain and loss terms into the G-P equation:

$$i\frac{\partial\psi}{\partial\tau} = -\frac{\partial^2\psi}{\partial\theta^2} + \alpha|\psi|^2\psi + V\psi + i(g-\gamma)\psi\,, \qquad (2)$$

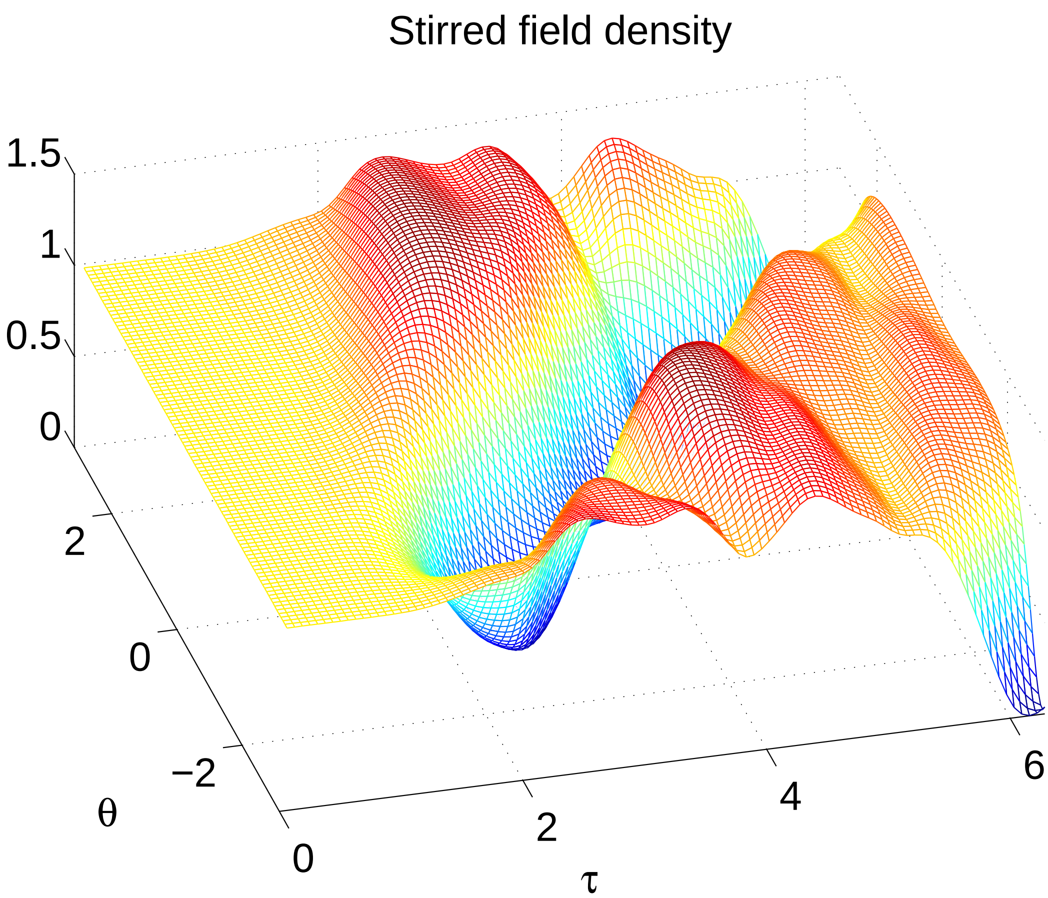
where V is the 'stirring' potential.

- **The gain mechanism g can be provided via stimulated emission from non-condensed atoms.**
- **The loss mechanism $\gamma(\tau,\theta)$ is due to an output coupler: a local Raman-tuned transition to a non-trapped state.**

Stirred, not shaken

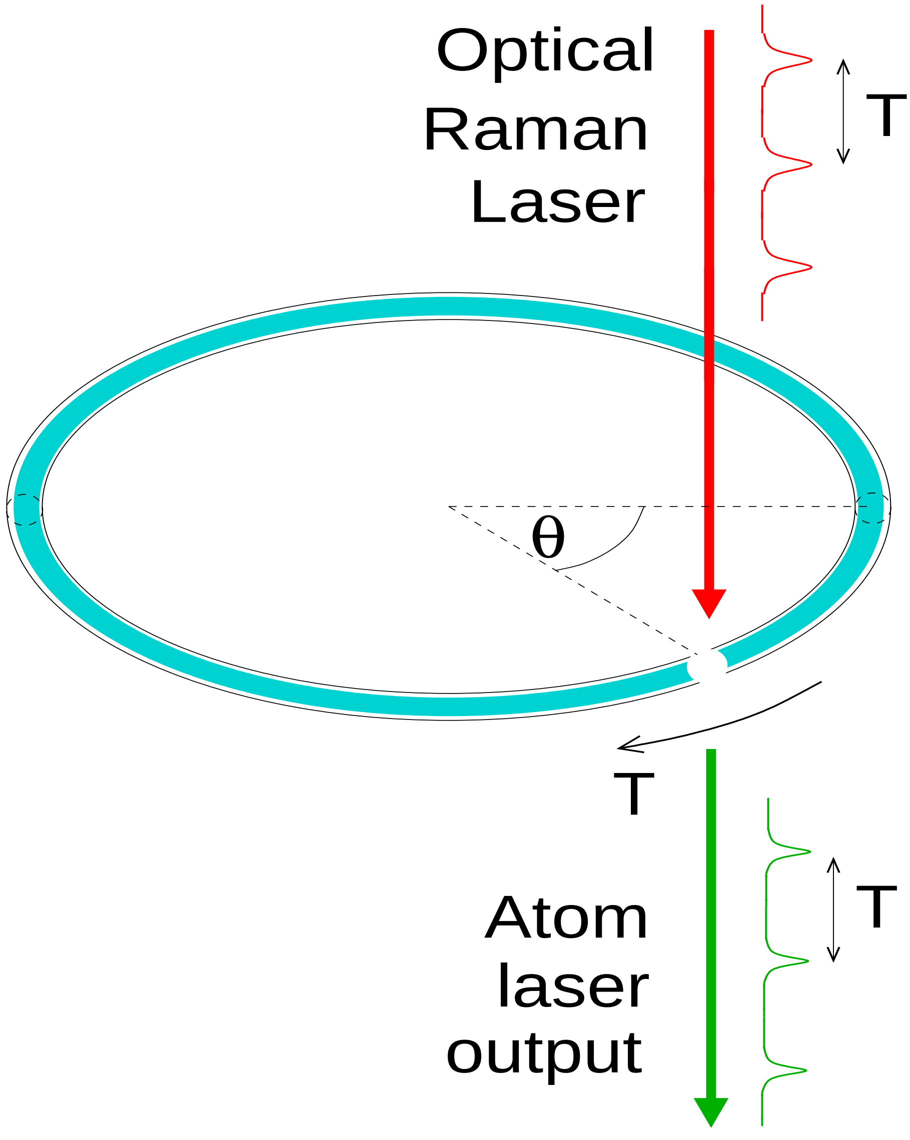
- We start by using a blue-detuned ‘stirring’ laser to form a moving potential hill.

- This repels the condensate from a localized region, which forms the phase singularity, and hence a soliton.



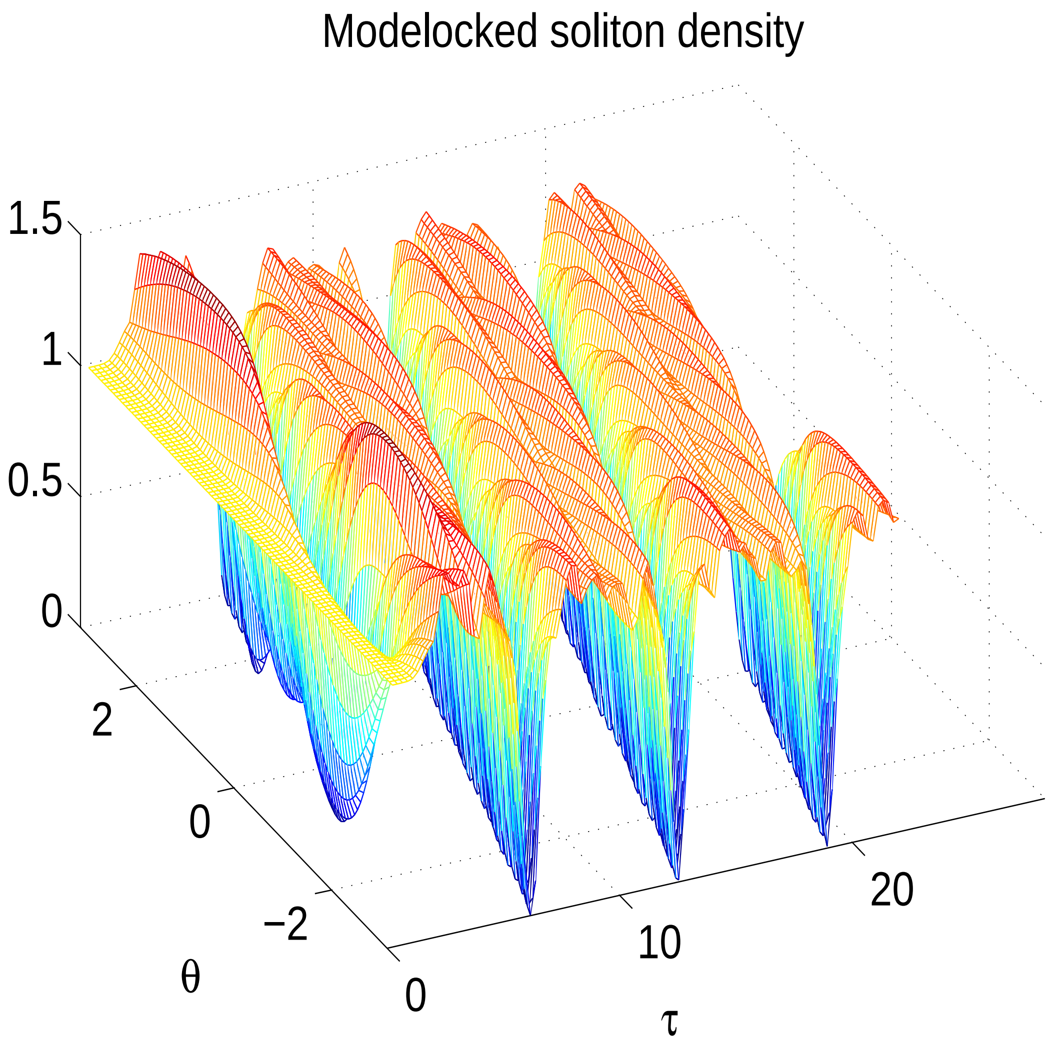
Dark Soliton Modelocking

Next, a periodic sequence of localized Raman laser pulses can be used to 'clean-up' or stabilize the dark soliton, while also producing an output pulse-train.



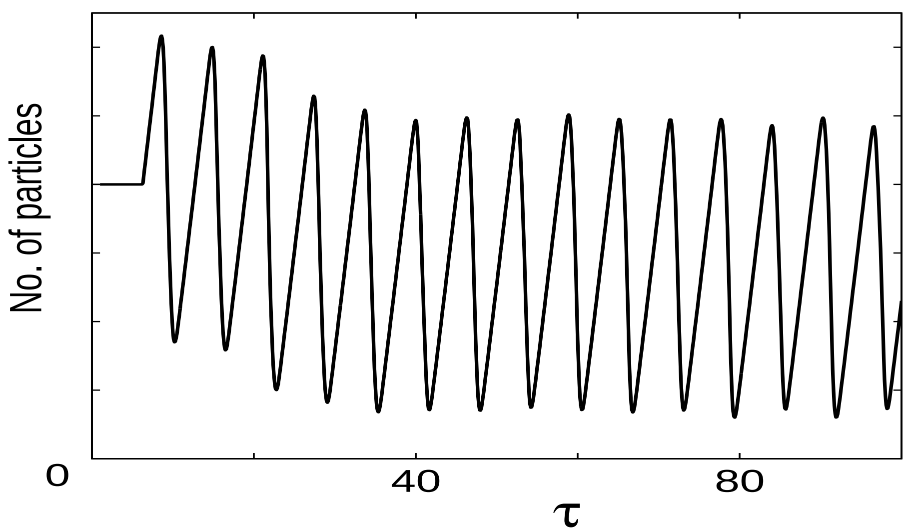
Evolution of the condensate

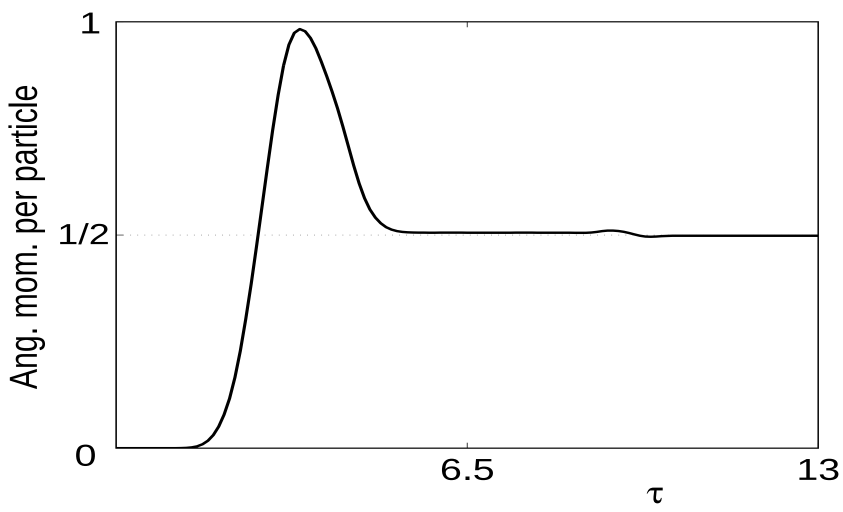
- The condensate is cleaned up, as phonons are removed by the mode-locker, to give a mode-locked output.



Stabilization

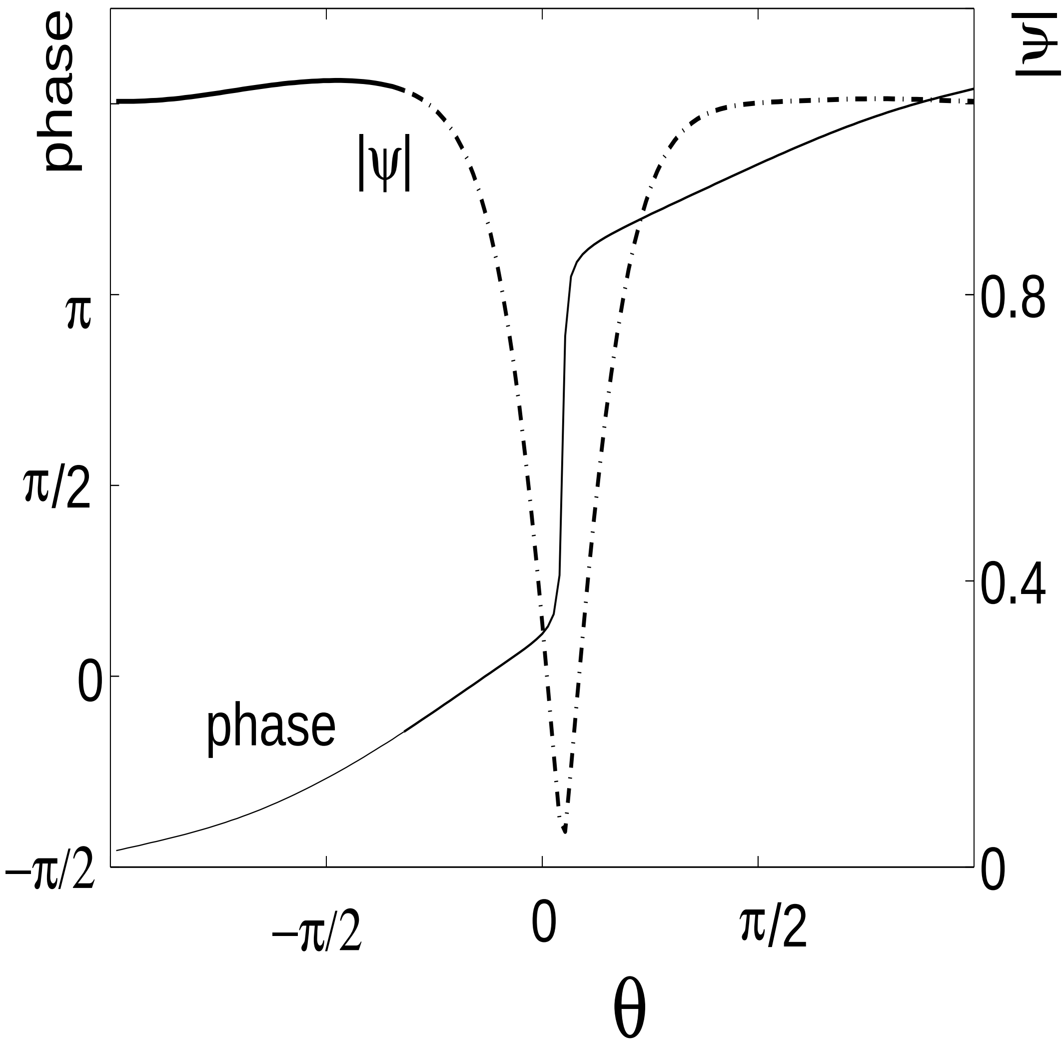
- BEC is stable: output-coupling is a nonlinear function of the atom number.





Stable mode-locked dark soliton

- The final result has an intensity 'hole', and stable phase from pulse to pulse.



SUMMARY

- We analyze stable, circulating dark solitons, in a toroidal atom laser .
- Lasing is achieved through super-saturated gain
- A periodic output coupler based on Raman transitions is used.
- The result is a dark soliton with angular momentum of $\hbar/2$ per atom.
- We have given a numerical treatment of soliton generation.[con-mat/90002389]
- **A modelocked atom laser is obtained.**

IV: SUPERCHEMISTRY

- **How do atom *waves* interact to make molecules?**

- In RAMAN PHOTOASSOCIATION: two atoms collide, absorb a photon and are stimulated to emit one, giving a ground molecular state.

- In nonlinear atom optics (BEC), describes coherent dimerization.

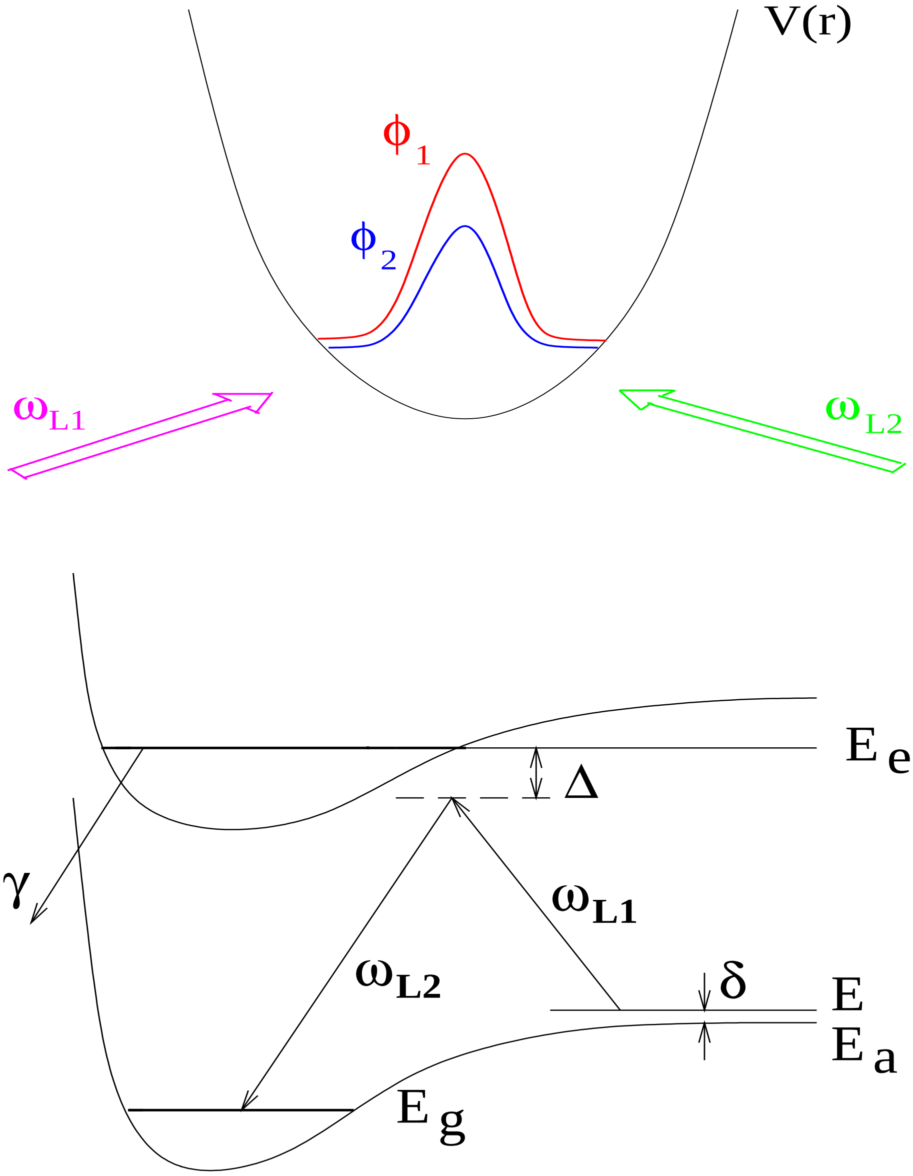
- **New physical effects resulting from this:**

- SUPERCHEMISTRY - stimulated nonlinear coherent chemistry

- SIMULTONS - coherent propagating atom-molecular solitons

EXPERIMENTAL TECHNIQUES

Superchemistry BEC simultons



[Heinzen et al., Science **287**, 986 (2000).]

Dynamics of atom-molecular BEC

Direct simulation of the mean-field theory equations:

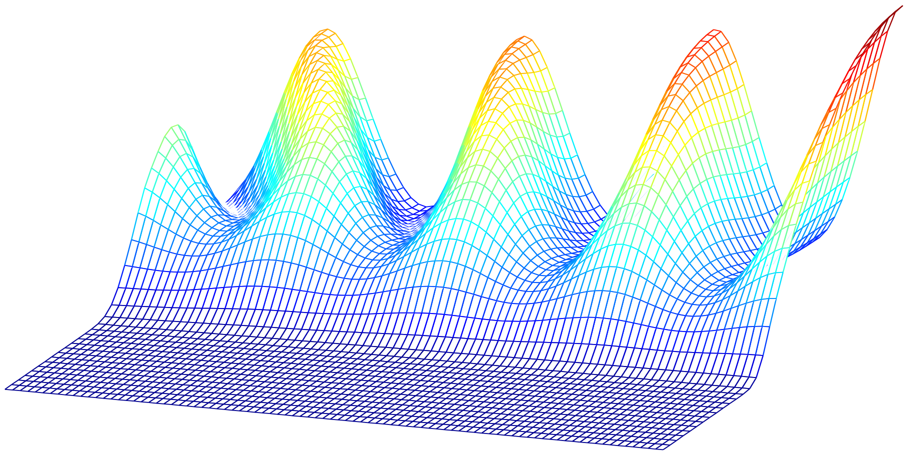
$$
\begin{aligned}
i\hbar\dot{\psi}_1 &= -\frac{\hbar^2}{2m_1}\nabla^2\psi_1 + V_1^c(\mathbf{x})\psi_1 + U_{11}^c|\psi_1|^2\psi_1 + \chi\psi_1^*\psi_2, \\
i\hbar\dot{\psi}_2 &= -\frac{\hbar^2}{2m_2}\nabla^2\psi_2 + V_2^c(\mathbf{x})\psi_2 + \frac{1}{2}\chi\psi_1^2,
\end{aligned}
$$

$$
\begin{aligned}
\frac{U_{11}}{\hbar} &\simeq \frac{4\pi\hbar a}{m_1} - \frac{\Omega_1^2}{2\sqrt{2}\Delta}|I_1|^2, \\
\frac{\chi}{\hbar} &\simeq -\frac{\Omega_1\Omega_2}{2\sqrt{2}\Delta} I_1 I_2, \\
I_1 &= \int dR\,[u_e(R)u_a^*(R)]\ , \\
I_2 &= \int dR\,[u_g(R)u_e^*(R)]\ .
\end{aligned}
$$

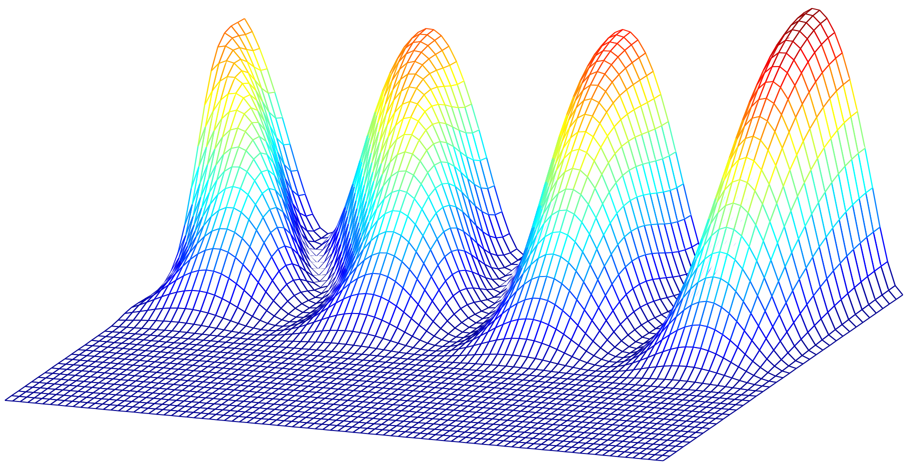
Here Ω_1 and Ω_2 are the Rabi frequencies, and Δ is the Raman detuning.

Superchemistry oscillations

ATOMIC BEC



MOLECULAR BEC



SUMMARY

- The simulations are carried out in two stages.

- In the first stage, we assume that only atomic species are present.

- In the second stage we switch on the coupling for molecule formation.

- Coherent stimulated emission into molecular BEC [Heinzen, Drummond et. al., (to appear), Phys. Rev. Lett.]

- Giant oscillations appear in the occupation number of the molecules.

- Bose-enhanced nonlinear quantum dynamics replaces the usual chemical kinetics: SUPERCHEMISTRY.

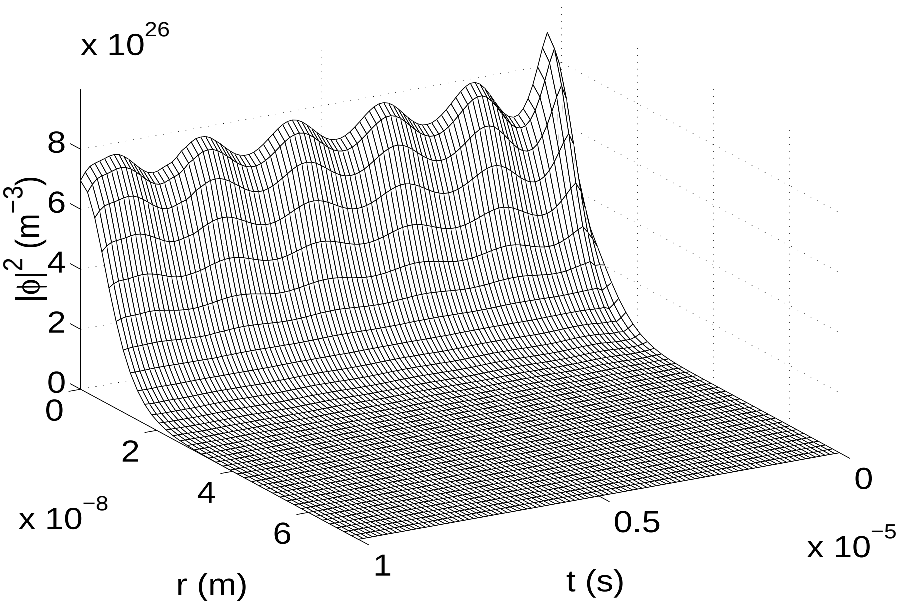
V: Classical solitons in 3D

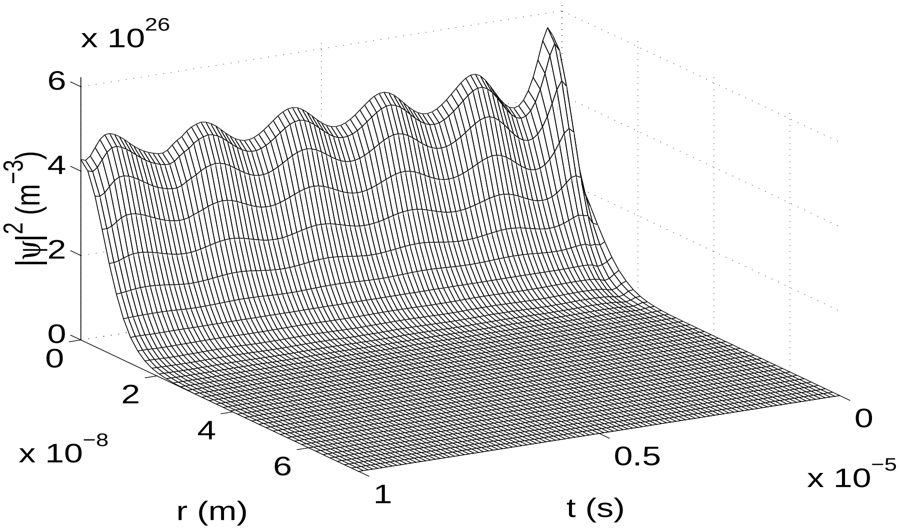
- **Can BEC matter become *stable* in free space?**

- These equations are known to have 3D solitons in photonics!

- Predicted by Malomed, Drummond et al (1998); observed by F. Wise (Cornell),1999.

Numerical simulations





Coherent or mean-field theory C-ansatz:

$$|\psi_C^{(N)}\rangle = \exp\left\{\int d^3\mathbf{x}\left[\psi_1(\mathbf{x})\hat{\Psi}_1^\dagger(\mathbf{x}) + \psi_2(\mathbf{x})\hat{\Psi}_2^\dagger(\mathbf{x})\right]\right\}|0\rangle\,.$$

- By varying $\psi_1(\mathbf{x})$ and $\psi_2(\mathbf{x})$, can get a soliton binding energy.
- The classical Hamiltonian is always bounded from below, by the classical soliton energy.
- P. D. Drummond, K. V. Kheruntsyan, and H. He, PRL **81**, 3055 (1988).

SUMMARY

- Can form three-dimensional atom-molecular BEC simultons.
- Also predicted to occur in photonics
- Verified experimentally in optics by F. Wise (Cornell)
- This is destabilised by atom-atom repulsion
- Coherent BEC nano-chemistry?
- **Stabilized nondiverging atom - molecular laser beams**

VI: QUANTUM SINGULARITIES

- Are there *localised* quantum eigenstates in 3D?

$$
\begin{aligned}
H &= H_0 + H_{int} + H_{self} \ , \\
H_0 &= \sum_i \int d^3\mathbf{x} \left[\frac{\hbar^2}{2m_i} |\nabla \hat{\Psi}_i(\mathbf{x})|^2 + V_i(\mathbf{x}) \hat{\Psi}_i^\dagger(\mathbf{x}) \hat{\Psi}_i(\mathbf{x}) \right] \\
H_{int} &= \chi \int d^3\mathbf{x} \hat{\Psi}_1^\dagger(\mathbf{x}) \hat{\Psi}_1^\dagger(\mathbf{x}) \hat{\Psi}_2(\mathbf{x}) + H.c., \\
H_{self} &= \sum_{i,j} \kappa^{(ij)} \int d^3\mathbf{x} \hat{\Psi}_i^\dagger(\mathbf{x}) \hat{\Psi}_j^\dagger(\mathbf{x}) \hat{\Psi}_j(\mathbf{x}) \hat{\Psi}_i(\mathbf{x}).
\end{aligned}
$$

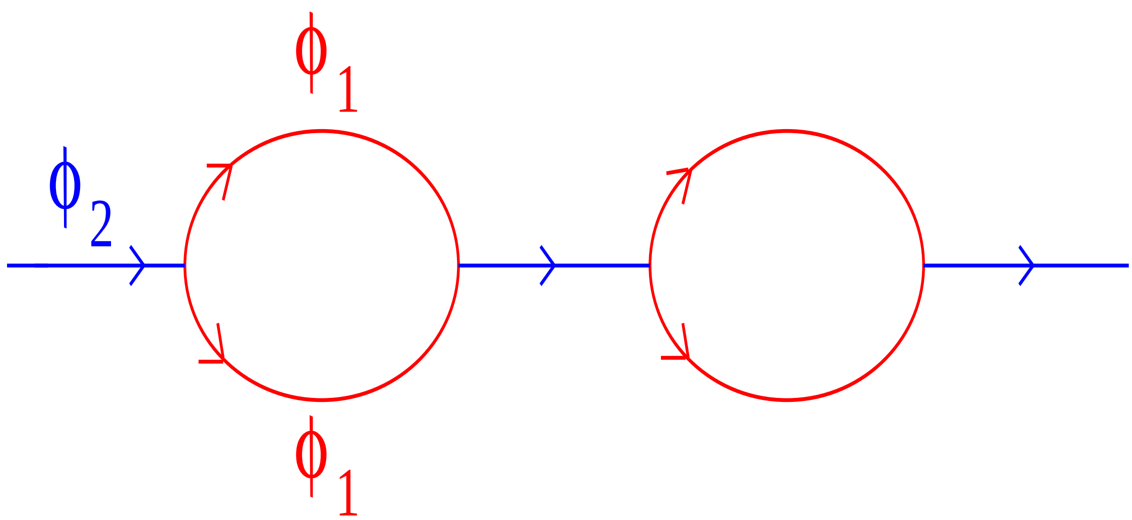
Two-particle quantum simultons

Simplest quantum soliton (simulton) $\left|\psi^{(2)}\right\rangle$ is a di-boson bound state ($N = 2$), which has the form of a superposition state:

$$\left[\int d^3\mathbf{x}\hat{\Psi}_2^\dagger(\mathbf{x}) + \int\int d^3\mathbf{x}d^3\mathbf{y}\ g(\mathbf{x}-\mathbf{y})\ \hat{\Psi}_1^\dagger(\mathbf{x})\hat{\Psi}_1^\dagger(\mathbf{y})\right]|0\rangle$$

- a 'dressed' molecule which exists in a superposition with a pair of atoms.

Similar solutions were discovered by T.D. Lee using two fermion fields, and no S-wave repulsion.



Properties of exact solutions

- Energy is bounded from below if $U_{11} > 0$ - unbounded if $U_{11} = 0$;

- Correlation function $g(\mathbf{r})$ has a point-like structure:

$$g(\mathbf{r}) = 0 \ , \quad \text{if} \quad |\mathbf{r}| > 0 \, , \quad g(0) = -\chi/(2U_{11}) \ .$$

- Exact binding energy per atom: $E_g^{(2)} = \Delta V - \chi^2/(4U_{11})$.

- $\Delta V = V_2^{(0)}/2 - V_1^{(0)}$.

- K. V. Kheruntsyan & P. D. Drummond, Phys. Rev. A **58**, 2488 (1988).

Independent Q-ansatz

The total N-particle ground state energy can be estimated using a variational approach:

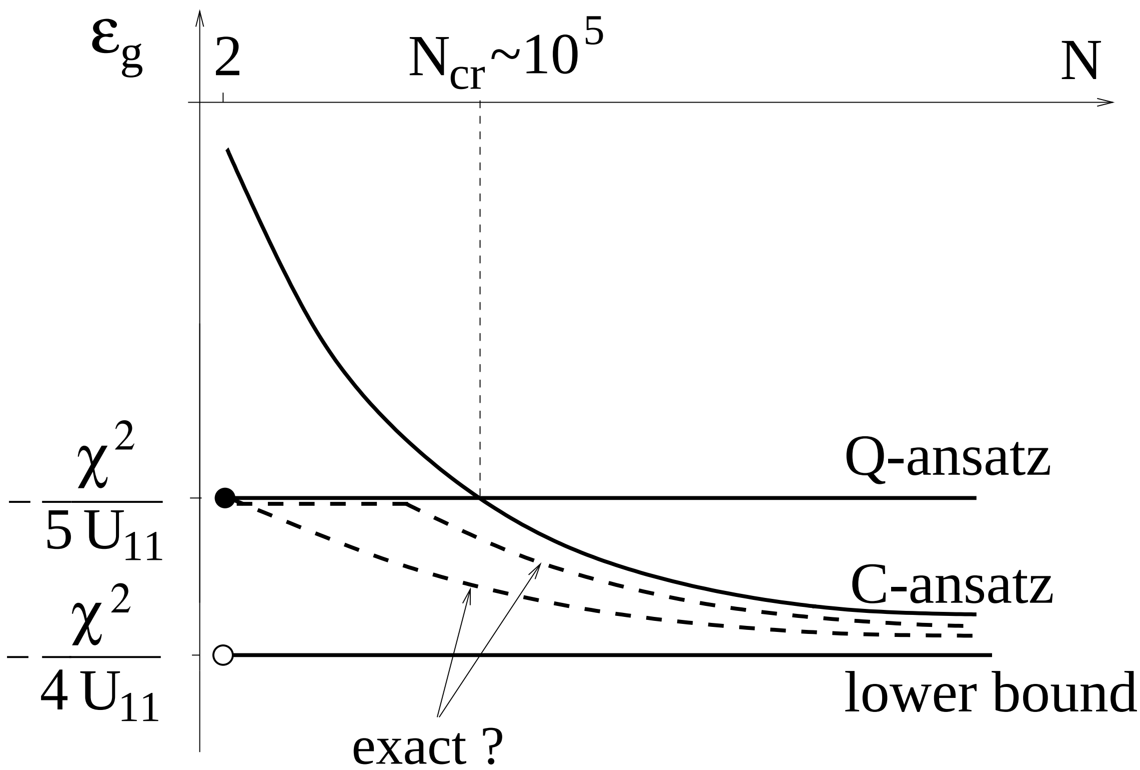
$$|\psi_Q^{(N)}\rangle = \left[\hat{b}^\dagger(0) + \int_{|k|=0}^{k_m} d^3\mathbf{k} G(\mathbf{k})\hat{a}^\dagger(\mathbf{k})\hat{a}^\dagger(-\mathbf{k})\right]^{N/2} |0\rangle \, .$$

- This corresponds to $N/2$ independent di-bosons or 'dressed' molecules;
- the energy upper bound is (for $k_m \gg [\chi m_1/(2\pi\hbar)]^2$): $E_Q^{(N)} = E_Q^{(2)} = \Delta V - \chi^2/(5U_{11})$.

Comparison of Q- vs C-ansatz

- The independent di-boson (Q-) and coherent (C-) ansatzs give different results; the coherent theory gives a better (lower) estimate for the ground state energy at $N \geq N_{cr}$, as $E_C^{(N)} \leq E_Q^{(N)}$.

- N_{cr} depends on a combination of momentum cutoff and density effects!



SUMMARY

- At low density, atoms couple to molecules in a particle-like way.

- For large momentum cutoff, these have a point-like structure.

- At large density, and large couplings χ, the coherent coupling of two entire condensates is dominant - just as in nonlinear optics.

- Can form three-dimensional atom-molecular BEC simultons.

- Could stabilize atom laser outputs; coherent BEC nano-chemistry?

- **A QUANTUM PHASE TRANSITION?**