

BEC & ATOM LASER THEORY AT UQ

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- **Quantum evaporative cooling** - what is the true state of a *real* BEC?
- **Superchemistry** - how do atom *waves* interact to make molecules?
- **Quantum solitons** - are there *localised* quantum eigenstates in 3D?
- **Classical solitons** - can BEC matter become *stable* in free space?
- **Mode-locking atom lasers** - how to make *coherent* atomic pulse-trains?
- **Atom wave-guides** - what happens to atoms interacting '*on a wire*' ?

I: Quantum evaporative cooling

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

A quantum simulation?..Impossible!

- “Can a quantum system be probabilistically simulated by a classical (probabilistic, I’d assume) universal computer? ...If you take the computer to be the classical kind I’ve described so far, (...) and there’re no changes in any laws, and there’s no hocus-pocus, the answer is certainly, No!” (Richard P. Feynman¹)
- “Hence the implications of Feynman’s argument seems to be that we really cannot simulate quantum dynamics on a local classical computer... Actual calculations involve only a few particles and very short propagations.” (David M. Ceperley²)
- “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. Ceperley³)

¹*Simulating Physics with Computers*, International Journal of Theoretical Physics **21**, 467 (1982)

²*The Simulation of Quantum Systems*, Address at receiving the Feenberg Medal

³*Lectures on Quantum Monte Carlo*, May 1996

+P representation

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

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

- $|\psi_i\rangle$ are coherent states of the atomic many-body operators
- $\mathcal{D}\psi_1, \mathcal{D}\psi_2$ are the functional integration measures
- $P(\psi_1, \psi_2)$ 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)

Results for optical solitons

- Quantum diffusion predicted for phase
- Quantum noise decreases in 'squeezed' quadratures
- First direct prediction of quantum effects in a soliton
- Typically have $10^8 - 10^9$ particles in 1000 modes; $\sim 10^{10000}$ modes available
- Rosenbluh and Shelby, IBM Almaden Laboratories: Observed quantum phase diffusion, squeezing
- Other experiments at NTT labs (Tokyo); MIT, Princeton, Erlangen

+P Equations

- the FPE leads to two stochastic phase-space equations:

$$\hbar \frac{\partial \psi_j}{\partial t} = [-\hbar^2 \nabla^2 / 2m + V(\mathbf{x}) - i\hbar \Gamma(\mathbf{x}) / 2 + U \psi_j \psi_{3-j}^* + \sqrt{i\hbar U} \xi_j(t, \mathbf{x})] \psi_j(t, \mathbf{x})$$

where:

- $j = 1, 2$; $m =$ atomic mass
- $V(\mathbf{x}) =$ trapping potential
- $\Gamma(\mathbf{x}) =$ loss rate
- $U =$ atom-atom coupling
- $\xi_j(t, \mathbf{x}) =$ stochastic term
- $\psi_2^* \psi_1 = \hat{\Psi}_2^+ \hat{\Psi}_1 =$ atom density

Summary

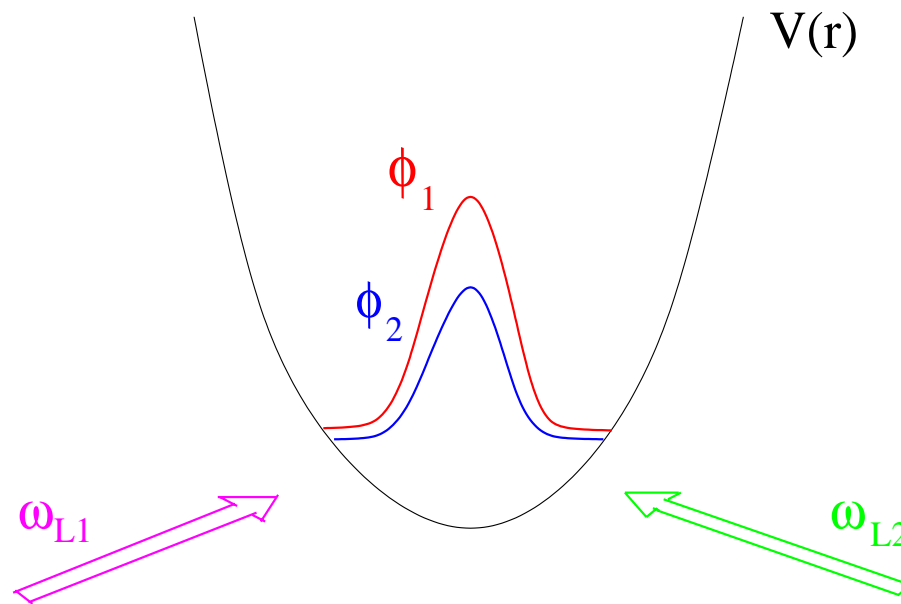
- first principles quantum simulation of BEC
- 10,000 atoms (initially) in 32000 trap modes; up to 200 atoms in condensate
- difficult - not impossible with classical computers
- physics: evaporative cooling with variable potential
- condensate can form in excited mode, with metastable vortices
- problems: sampling error increases with time; basis set needs to be refined - an initial coherent state does not remain a coherent state.

II: SUPERCHEMISTRY

- **How do atom waves interact to make molecules??**
- We consider a degenerate or nondegenerate case.
- 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

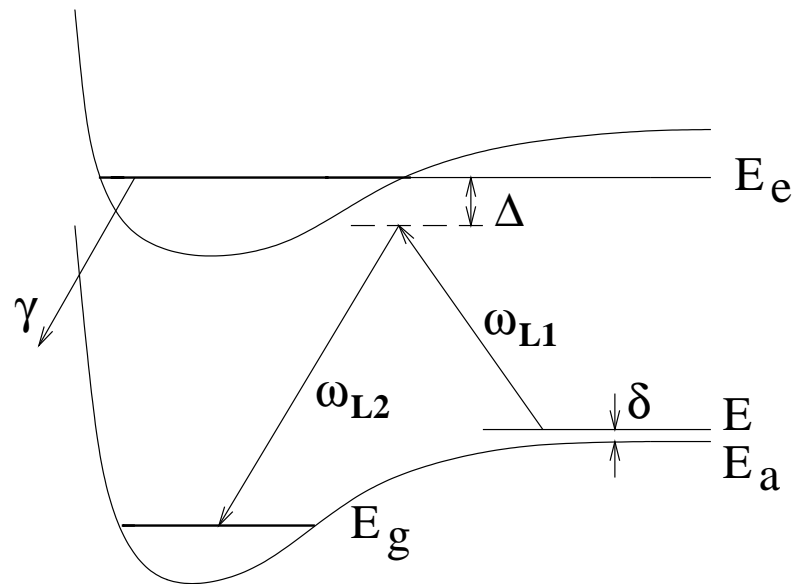
EXPERIMENTAL TECHNIQUES

Superchemistry BEC simultons



- Photo-association coupling of two atoms to one molecule

Raman photoassociation



- Nonresonant coupling with two coherent lasers (D. Heinzen, Texas).

How does it work?

- In **PHOTOASSOCIATION**: a pair of free atoms collide AND absorb a photon from a laser beam, giving an excited molecular state.
- In **RAMAN PHOTOASSOCIATION**: two atoms collide, absorb a photon and are stimulated to emit one, giving a ground molecular state.
- Photoassociative spectroscopy with cold atoms has proven to be a powerful tool for probing molecular vibrational levels.
- Raman photoassociation can change the atomic scattering length.
- Less loss-prone than Feshbach resonance (Ketterle, Heinzen, Wieman).

Coherent dynamics of atom-molecular bec

Direct simulation of the mean-field theory equations, in the presence of trap potentials:

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

where parameters are calculated for the case of Rubidium dimerization using typical laser intensities and data from the Heinzen experiment. Find non-Arrhenius behaviour - giant nonlinear oscillations.

Photo-association effective couplings

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

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

SIMULATIONS

- 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 χ for molecule formation.
- We include additional spontaneous decay terms.
- Giant oscillations appear in the occupation number of the molecules.
- Bose-enhanced nonlinear quantum dynamics replaces the usual chemical kinetics: **SUPERCHEMISTRY**.

III: QUANTUM SOLITONS in 3D

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

$$H = H_0 + H_{int} + H_{self} ,$$

$$H_0 = \sum_i \int d^3\mathbf{x} \left[\frac{\hbar^2}{2m_i} |\nabla \hat{\Psi}_i(\mathbf{x})|^2 + V_i(\mathbf{x}) \hat{\Psi}_i^\dagger(\mathbf{x}) \hat{\Psi}_i(\mathbf{x}) \right] ,$$

$$H_{int} = \chi \int d^3\mathbf{x} \hat{\Psi}_1^\dagger(\mathbf{x}) \hat{\Psi}_2^\dagger(\mathbf{x}) \hat{\Psi}_3(\mathbf{x}) + H.c. ,$$

$$H_{self} = \sum_{i,j} \kappa^{(ij)} \int d^3\mathbf{x} \hat{\Psi}_i^\dagger(\mathbf{x}) \hat{\Psi}_j^\dagger(\mathbf{x}) \hat{\Psi}_j(\mathbf{x}) \hat{\Psi}_i(\mathbf{x}) .$$

Energy eigenstates

–or **quantum solitons (simultons)**, must simultaneously be the eigenstates of

$$\hat{N} = \int d^3\mathbf{x} \left[|\hat{\Psi}_1|^2 + 2|\hat{\Psi}_2|^2 \right] = \hat{N}_1 + 2\hat{N}_2,$$

conserving the **generalized particle number** N (total number of atoms if we count each molecule as two atoms).

Simplified version:

- in free space (no trap potentials);
- no momentum cutoff.

Two-particle quantum solitons

Simplest quantum soliton (simulton) is a di-boson bound state ($N = 2$), which has the form of a **superposition state**:

$$|\psi^{(2)}\rangle = \left[\int d^3\mathbf{x} \hat{\Psi}_2^\dagger(\mathbf{x}) + \int \int d^3\mathbf{x} d^3\mathbf{y} g(\mathbf{x} - \mathbf{y}) \hat{\Psi}_1^\dagger(\mathbf{x}) \hat{\Psi}_1^\dagger(\mathbf{y}) \right] |0\rangle$$

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

Solutions of similar form were first discovered by T.D. Lee in meson physics (except using two fermion fields, and no S-wave repulsion)

- S. Schweber, Relativistic Quantum Field Theory.

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:

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

- **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).

N -particle exact solution

Even N -particle eigenstates have the form of $N/2$ independent di-bosons:

$$|\psi^{(N)}\rangle = \left[\int d^3\mathbf{x} \hat{\Psi}_2^\dagger(\mathbf{x}) + \int \int d^3\mathbf{x} d^3\mathbf{y} g(\mathbf{x} - \mathbf{y}) \hat{\Psi}_1^\dagger(\mathbf{x}) \hat{\Psi}_1^\dagger(\mathbf{y}) \right]^{N/2} |0\rangle.$$

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

- In the limit $U_{11} \rightarrow 0$, we obtain singularity and energy collapse;
- This is in contrast to the known mean-field behavior of the classical energy, which is rigorously bounded from below.

QUANTUM SIMULTONS WITH CUTOFF

We introduce a momentum cutoff ($k_m \sim 2\pi/a$):

$$|\psi_Q^{(2)}\rangle = \left[\hat{b}^\dagger(0) + \int_0^{k_m} d^3\mathbf{k} G(\mathbf{k}) \hat{a}^\dagger(\mathbf{k}) \hat{a}^\dagger(-\mathbf{k}) \right] |0\rangle,$$

where \hat{a} and \hat{b} are Fourier components of $\hat{\Psi}_1$ and $\hat{\Psi}_2$.

- Quantum (di-boson) soliton acquires finite radius;
- the binding energy is (for $k_m \gg [\chi m_1 / (2\pi\hbar)]^2$) is:
 $E_Q^{(2)} = \Delta V - \chi^2 / (5U_{11})$.

Approximate N -particle solutions: independent Q-ansatz

The total binding or 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 $k_m \gg [\chi m_1 / (2\pi\hbar)]^2$):
 $E_Q^{(N)} = E_Q^{(2)} = \Delta V - \chi^2 / (5U_{11})$.

IV: Classical solitons in 3D

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

The above Q-ansatz, **at finite** k_m , does not give the lowest possible energy. To show this, we consider a coherent or mean-field theory (MFT) 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 lower energy than previously.
- The calculation makes use of the known result that the classical Hamiltonian is always bounded from below, and the bound is given by the classical soliton energy.

Energy estimate by Gaussian C-ansatz

- Choosing $\psi_j(\mathbf{x}) = (-1)^{j-1} g_j N^2 [2/(\pi s_j)]^{3/4} \exp(-|\mathbf{x}|^2 N^2/s_j)$ results in:

$$E_C^{(N)}/\hbar = N^2 \left(\frac{3\hbar}{2m_1} \right) \left[\frac{g_1^2}{s_1} + \frac{g_2^2}{2s_2} - \frac{\tilde{\chi} g_1^2 g_2 s_2^{3/4}}{(s_1 + 2s_2)^{3/2}} \right] + N^4 \tilde{U} g_1^4 s_1^{-3/2} + \rho g_2^2 ,$$

- where: $\tilde{\chi} = 2^{5/2} (2/\pi)^{3/4} m \chi / (3\hbar)$ and: $\tilde{U} = 2^{-5/2} (2/\pi)^{3/2} U_{11}$.
- Minimize $E_C^{(N)}$, under the constraint of a fixed N .
- P. D. Drummond, K. V. Kheruntsyan, and H. He, PRL **81**, 3055 (1988).

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!
- For $m_1 \sim 10^{-25} \text{ kg}$, $\chi/\hbar \sim 10^{-6} \text{ m}^{3/2}/\text{sec}$, $a \sim 2\pi \text{ nm}$, so that $U_{11}/\hbar \simeq 8 \times 10^{-17} \text{ m}^3/\text{s}$, and a cutoff at $k_m = 2\pi/a \sim 1 \text{ nm}^{-1}$, we obtain:

$$N_{cr} \sim 1.4 \times 10^5.$$

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.
- Call this a type of **superchemistry** in BEC.
- Can form three-dimensional atom-molecular BEC **simultons**.
- Could **stabilize** atom laser outputs; coherent BEC nano-chemistry?

V: Mode-locking atom lasers

- **How can we make *coherent* atomic pulse-trains?**
- The laser is constructed as a torus using magnetic trapping techniques.
- Modelocking is achieved by using a periodic output coupler to generate a dark soliton with angular momentum of $\hbar/2$.
- This results in a periodically replicating coherent field inside the torus.
- The soliton is started by laser stirring
- **The mode-locking process leads to a stable dark soliton with fractional angular momentum quantum number.**

Dimensionless G-P equation

A dimensionless form of the 1D G-P equation:

$$i\frac{\partial\psi}{\partial\tau} = -\frac{\partial^2\psi}{\partial\theta^2} + V\psi + \alpha|\psi|^2\psi. \quad (1)$$

The normalization and periodicity conditions are now:

$$\int_0^{2\pi} d\theta \psi^* \psi = 2\pi, \\ \psi(\theta + 2\pi, \tau) = \psi(\theta, \tau). \quad (2)$$

Uniform vortex

A uniform vortex state with angular momentum l has the condensate wave function

$$\psi_l(\theta, \tau) = e^{-i\nu_l\tau + il\theta} \quad (3)$$

where l must be an integer, in order to satisfy the boundary condition. The equation of motion gives

$$\nu_l = \alpha + l. \quad (4)$$

The energy and momentum per particle of the uniform vortex state are

$$\begin{aligned} W &= \alpha/2 + l^2, \\ J &= l \quad (l = 1, 2, 3, \dots). \end{aligned} \quad (5)$$

Soliton solutions

The one-dimensional NLSE is known to be classically integrable, and to have periodic soliton solutions that correspond to localized disturbances traveling around the circumference of the torus. For a soliton solution, put

$$\psi(\theta, \tau) = f(\theta - v\tau)e^{i\eta(\theta, \tau)}, \quad (6)$$

where v is an arbitrary real parameter, corresponding to the soliton velocity. In general, a continuous set of velocities is possible. Complex values of f correspond to grey solitons, having non-integer velocities.

- **Real values of f correspond to dark and bright solitons, having integer values of v .**

Dark and Bright Solitons

In the case of a real envelope function the boundary condition demands

$$\begin{aligned} f(\bar{\theta} + 2\pi) &= (-1)^{2l} f(\bar{\theta}), \\ \eta(\theta + 2\pi, \tau) &= \eta(\theta, \tau) + 2\pi l, \end{aligned} \quad (7)$$

where $\bar{\theta} \equiv \theta - v\tau$, and $l = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \pm 2, \dots$. Assume the form

$$\eta(\theta, \tau) = l(\theta - v\tau) - \omega\tau, \quad (8)$$

where ω is an arbitrary real parameter. This satisfies the boundary condition. For f to be real, the angular momentum is

$$J = l = v/2. \quad (9)$$

Exact Dark Soliton Solutions

We consider the case $\alpha > 0$.

The explicit solution in terms of the Jacobi elliptic function is:

$$f(\bar{\theta}) = f_2 sn \left(f_1 \sqrt{\frac{\alpha}{2}} (\bar{\theta} - \pi/s) \right). \quad (10)$$

- **This is an exact solution, with half-integer angular momentum.**

Tanh with a twist

For large α , we find the approximate solution

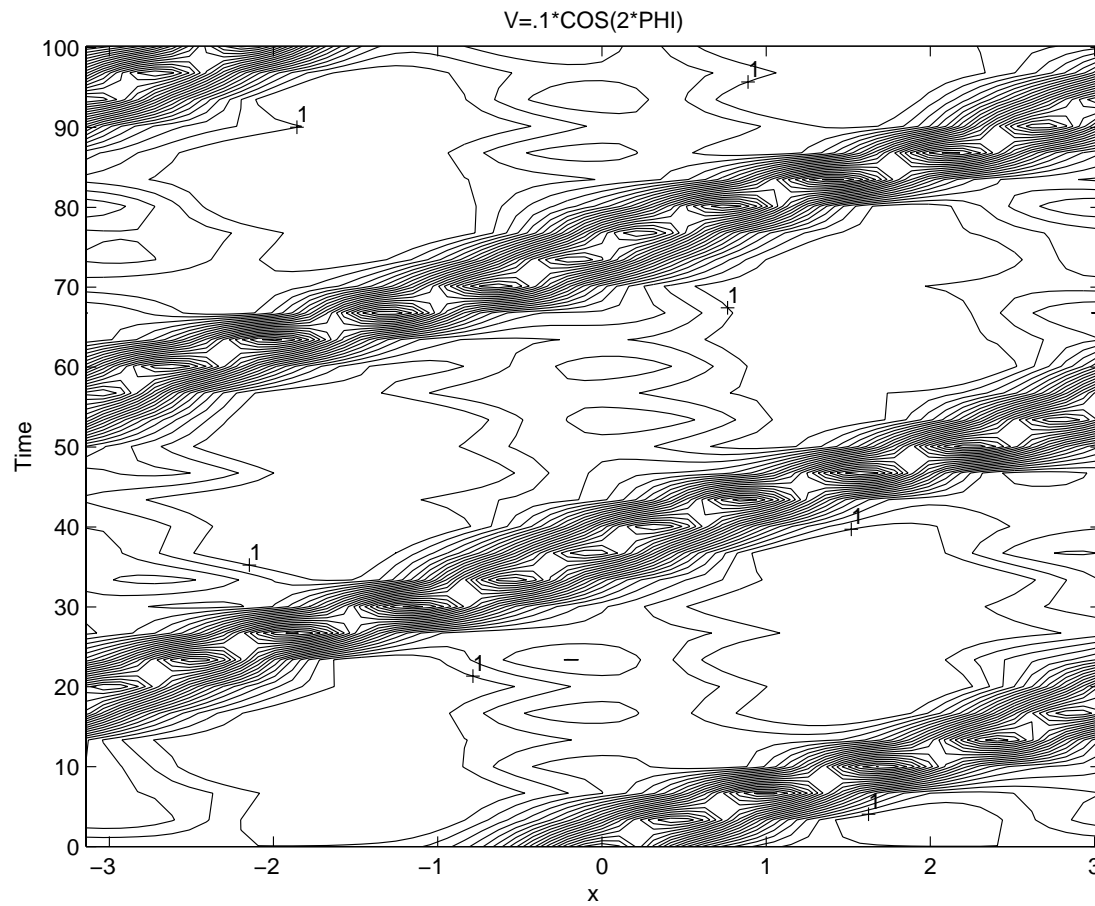
$$f(\bar{\theta}) = \sqrt{\frac{\beta}{\alpha}} \tanh \left(\sqrt{\frac{\beta}{2}} (\bar{\theta} - \pi/s) \right) . \quad (11)$$

Where:

$$\beta \simeq \alpha \left(1 + \frac{1}{2\pi} \sqrt{\frac{2}{\alpha}} \right) . \quad (12)$$

- **To form the solution, the sign change in the tanh is compensated for by an ODD number of π phase-rotations or ‘twists’ due to the condensate orbital angular momentum.**

Stability in a non-symmetric trap



Mode-locked atom laser

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

$$i\frac{\partial\psi}{\partial\tau} = -\frac{\partial^2\psi}{\partial\theta^2} + \alpha|\psi|^2\psi + V\psi + i(g - \gamma)\psi, \quad (13)$$

where V is the ‘stirring’ potential.

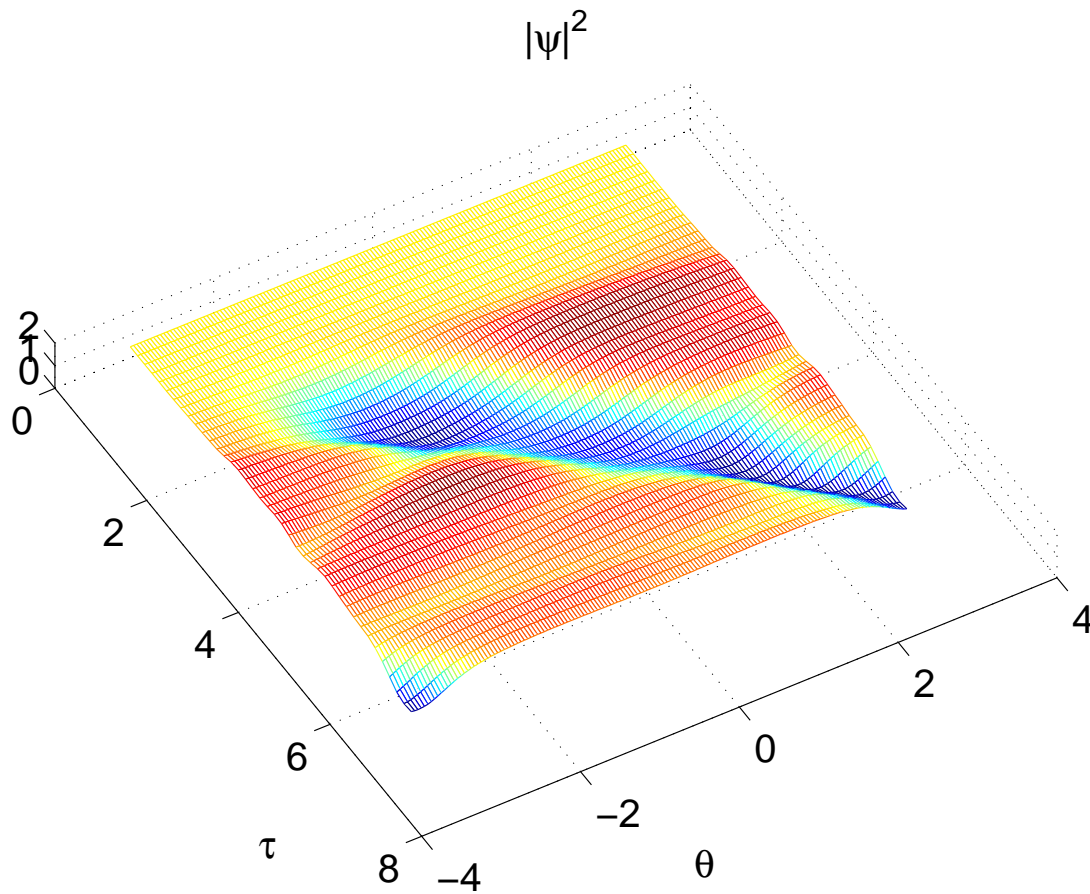
- **The gain mechanism g can be provided via stimulated emission from non-condensed atoms that are continuously loaded into the trap.**
- **The loss mechanism γ is due to an output coupler, like a local Raman-tuned transition to a non-trapped state of the atoms.**

Shaken, not stirred?

- We start by assuming that a blue-detuned ‘stirring’ laser is employed to form a moving, positive potential hill.
- This repels the condensate, forming the phase singularity.
- The potential hill is moved, accelerating the condensate in the required direction, to form a moving tanh-like excitation.
- To give definite results, consider the stirring potential in Fig. (3), chosen to be localized in time, but moving at the desired soliton velocity:

$$V(\theta, \tau) = V_0 e^{-(\pi + \theta - \tau)^2 / \sigma_1^2} e^{-(\tau - \pi)^4 / \sigma_2^4}. \quad (14)$$

Stirred Field



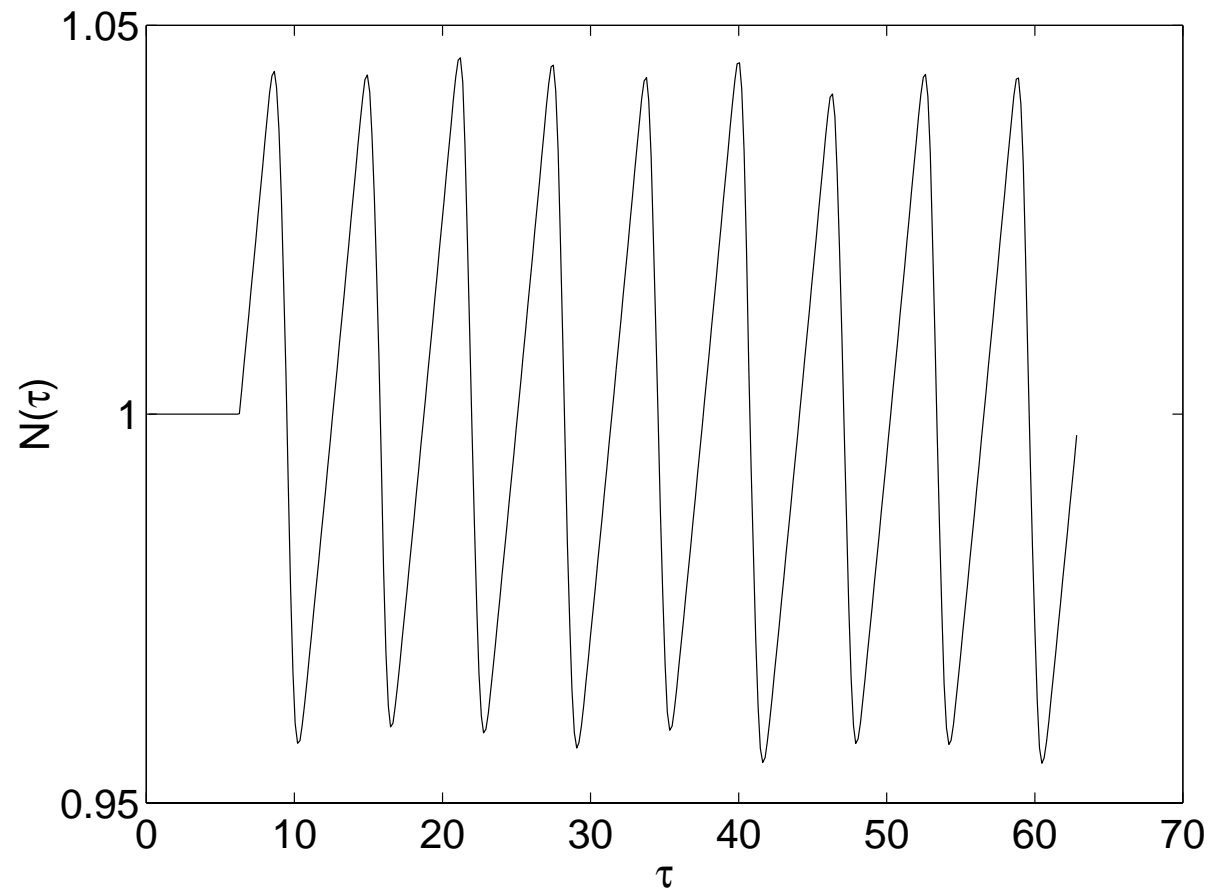
Dark Soliton Modelocking

If the mean atom number in the condensate increases, the hole shrinks in diameter, thus increasing the out-coupling efficiency and losses. On the other hand, a decrease in atom number will increase the hole diameter. This reduces the output coupler efficiency, and therefore decreases the losses.

The same mechanism also gives rise to a stable condensate phase and velocity, which otherwise could vary, allowing a grey soliton to form by continuous deformation of the initial dark soliton phase.

- **The mean atom number in the entire BEC is stabilized by the fact that the output-coupling efficiency is a nonlinear function of the hole diameter, and hence of the atom number.**

Stabilization process



Conclusion

- The calculations given here demonstrate how to generate stable, circulating dark solitons, in a toroidal atom laser .
- Lasing is achieved by using the super-saturated gain model.
- A periodic output coupler based on Raman transitions is used.
- The result is the generation of a dark soliton with angular momentum of $\hbar/2$ per atom.
- We have given a numerical treatment of soliton generation.
- **A stable, mode-locked Bose-Einstein condensate with a fractional angular momentum quantum number is possible.**

VI: Atom wave-guides

- **What happens to atoms interacting ‘*on a wire*’ ?**
- Not enough time to show everything!