Theory of Coherent Photoassociation of the Bose Einstein Condensates

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We study coherent photoassociation, phenomenon analogous to coherent optical transient in a few-level system, which takes place in photoassociation of an atomic Bose-Einstein condensate, unlike in a nondegenerate gas. We describe the interacting condensates using the Gross-Pitaevskii formalism. The resulting equations are analyzed numerically, as well as theoretically. We describe the tools we developed in achieving these goals: a novel numerical method for the systems of linear and nonlinear hamiltonian equations, *DS-method*; and the modification of the Zakharov stability analysis, applied to our particular problem of two coupled Bose-Einstein condensates. We

analyze the properties of the solutions to a coupled problem in purely theoretical fashion for the cases of free and trapped condensates. We deduce general properties of the trapped solutions, in particular, their structural stability, and the adiabatic approximation of the initial problem. The structural stability, which is proven mathematically, has many repercusions to the possible interpretations of the present experimental results, and may influnce further theoretical study of the photoassociation phenomenon in the atomic Bose-Einstein condensate.

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to Otto and Kodi

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Everybody, thank you.

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Appendix A

Proof: A collapse of η to zero is not possible

In Sec.() we have derived an ordinary differential equation for the functional η,

$$\ddot{\eta} + 4\eta = DE + (4 - D)E_0 + \frac{D\delta}{2} \langle\psi|\psi\rangle \,. \tag{A.1}$$

This ordinary differential equation describes a nonautonomous system, because of the two terms on the right-hand side, E_0 and $\langle\psi|\psi\rangle$. These cannot be expressed as the functions of η, rather they are the functions of the density distributions φ and ψ. So, in order to find the evolution of $\eta = \eta(\tau)$ one has to follow the evolution of the fields $\varphi(\tau)$ and $\psi(\tau)$, and then along such a trajectory calculate $E_0(\tau) = E_0(\varphi(\tau), \psi(\tau))$, and $\langle\psi(\tau)|\psi(\tau)\rangle$.

However, while our knowledge of η is limited, we can still deduce some of its properties. Most important of these are

- $\exists\tau^* > 0$, determined by the evolution of φ and ψ, such that $\eta(\tau), \dot{\eta}(\tau)$ and $\ddot{\eta}(\tau)$ are continuous on $[0, \tau^*\rangle$,
- for such τ^*, the limits $\eta(\tau)$, $\dot{\eta}(\tau)$ and $\ddot{\eta}(\tau)$ exist $\forall\tau \in [0, \tau^*]$.

These follow from the definition of η as a weighted integral over the distributions φ and ψ , which are continuous on $[0, \tau^*\rangle$. Same holds for the average value of the operator $\mathbf{x}\,\nabla$ over the distributions φ and ψ, thus making $\dot{\eta}$ continuous. The $\ddot{\eta}$ is continuous, as well, by virtue of the Eq. (A.1). The latter are continuous everywhere except at the collapse point $\eta = 0$, however they are defined there in the sense that their limits exist.

These statements *per se* allow a collapse of η to zero, but they limit its first occurance to the time τ^*, which can be either finite or infinite.

Applying the Heisenberg's uncertainty relationships to E_0 yields,

$$E_0\,\eta \geq \frac{D}{64}\,. \tag{A.2}$$

Finally, using the normalizability of the distribution ψ, that is $0 \leq \langle\psi|\psi\rangle \leq 1$, Eq. (A.1) can be rewritten as an inequality

$$\ddot{\eta} + 4\eta \geq A + \frac{K}{\eta}, \tag{A.3}$$

with the initial condition $\eta(0) > 0$, and parameters $K = (4 - D)D/64 > 0$ and $A = DE - D|\delta|/2 \in \Re$.

We now demonstrate that given the inequality (A.3) and the properties of functional $\eta = \eta(\tau)$ listed above, the collapse of η to zero is not possible. We use *Reductio ad absurdum.*

So we assume opposite. Say, the collapse point $\eta = 0$ has been reached. Consider now that η and its time derivatives were continuous during the collapse, and that η is not identically equal to zero, and observe the inequality

$\ddot{\eta}$ as the function of η satisfies at the collapse point $\eta = 0$,

$$\ddot{\eta}(0) = +\infty = \dot{\eta}(0)\,\frac{d\dot{\eta}}{d\eta}(0) > 0. \tag{A.4}$$

By the initial assumption, η and its derivatives are well defined everywhere, including at the collapse point so the above expression is meaningful.

The inequality (A.4) together with the continuity assumption implies an existence of a finite closed neigborhood $[0, \Delta\eta]$, such that (i) $\dot{\eta} < 0$, and (ii) $\frac{d\dot{\eta}}{d\eta} < 0$, both hold.

To see that $d\dot{\eta} > 0$ holds in the neighborhood $[0, \Delta\eta]$, let us rewrite $d\dot{\eta} = \ddot{\eta}dt$. Here $dt > 0$ is an infinitesimal time increment along the collapse path, and $\ddot{\eta} > 0$ by the assumption used in the construction of the neighborhood. Thus, (ii) implies that $d\eta \leq 0$ along the collapse path in the neighborhood $[0, \Delta\eta]$, as one would expect. An example of a hypothetical collapse path satisfying these conditions is plotted in Fig. (A.1).

We now take inequality (A.3), multiply both sides by $d\eta$, $d\eta \leq 0$, and integrate along the collapse path from $\eta = \Delta\eta$ to $\eta = 0$. This yields

$$\frac{1}{2}\dot{\eta}^2\,|_{\eta=\Delta\eta}^{\eta=0} \leq \left(\ln\eta + A\eta - 2\eta^2\right)|_{\eta=\Delta\eta}^{\eta=0} \tag{A.5}$$

Right-hand side of the inequality can be readily evaluated and is $-\infty$, forcing

$$\frac{1}{2}\dot{\eta}^2(0) - \frac{1}{2}\dot{\eta}^2(\Delta\eta) \leq -\infty. \tag{A.6}$$

Independently of the value of $\dot{\eta}(0)^2$ this requires

$$+\infty \leq \dot{\eta}^2(\Delta\eta). \tag{A.7}$$

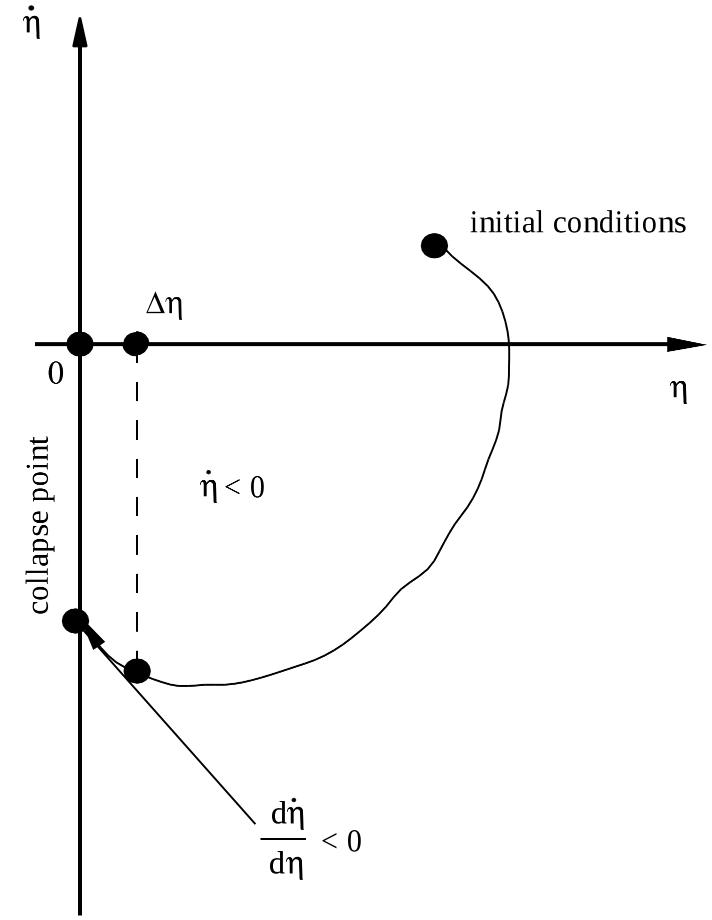

Fig. A.1: An anticipated path of collapse in $\{\eta, \dot{\eta}\}$ space.

This result, which is valid for a range of values of $\Delta\eta$ contradicts the initial assumption that η and its time derivates are continuos functions prior to the collapse moment.

This finishes the proof and we conclude that $\eta = \eta(\tau)$ whose second time derivative $\ddot{\eta}$ is described by both Eq.(A.1) and inequality (A.3) and given the initial condition $\eta(0) > 0$, never reaches the value $\eta = 0$.

Appendix B

Introduction to DS-method for numerical solving of the systems of Schrödinger Equations

The DS-method originates in the paper of M. Koštrun and J. Javanainen, Ref. [1], regarding one possible replacement for the split-step class of methods, Ref. [2]. The acronym "DS" comes from "Dirac" or "Dual Stepping" method, indicating the contribution of interaction picture (initially created by Dirac) and the nature of the method, that is opposite of the splitting.

The idea is to bring an initial value problem,

$$\begin{aligned} & i\tfrac{\partial\varphi}{\partial t} = H_0\varphi + W\left[t,\varphi\right], \\ & \varphi(0,x) = f(x), x \in \langle -L, L\rangle\,. \end{aligned} \tag{B.1}$$

using a sequence of linear transformations to the form that is formally solvable using an ODE integration formula. Here H_0 is a Hamiltonian, $H_0 = -\frac{1}{2}\nabla^2 + V_0(\vec{x})$, linear and time independent operator, and W is a contact interaction in the sense that

$$W\left[t,\varphi\right](x) = W\left(t, x, \varphi(x,t)\right). \tag{B.2}$$

The initial transformation corresponds to a so called interaction picture of quantum mechanics, e.g. see Ref. [3]. This formally removes a linear time-independent operator H_0 from Eq.(B.1) , to yield a familiar expression

$$\varphi(t) = e^{-iH_0 t}\tilde{\varphi}(t) = u_0(t)\tilde{\varphi}(t). \quad \text{(B.3)}$$

The Schrödinger equation for the new wave function $\tilde{\varphi}(t,x)$ becomes:

$$i\frac{\partial\tilde{\varphi}}{\partial t} = e^{iH_0 t} W\left[t, e^{-iH_0 t}\tilde{\varphi}\right]. \quad \text{(B.4)}$$

Next step is to divide the time domain $[0,T]$ in the N intervals of the equal length $\Delta T = \frac{T}{N}$. On each of the intervals, $[t_k, t_{k+1}]$, $k = 0 \ldots N-1$, we apply a local transformation result of which is a new wave function $\hat{\varphi}(\tau)$ such that

$$\hat{\varphi}(\tau) = e^{-iH_0 t_k}\tilde{\varphi}(t_k + \tau). \quad \text{(B.5)}$$

The original problem Eq.(B.1) is by virtue of these two transformations conviniently modified to the following form

$$i\frac{\partial\hat{\varphi}(\tau)}{\partial\tau} = e^{iH_0\tau} W\left[t_k + \tau, e^{-iH_0\tau}\hat{\varphi}\right], \text{ for } \tau \in [0, \Delta T]. \text{ and } k = 0 \ldots N-1 \quad \text{(B.6)}$$

The initial condition for $\tau = 0$ on the $k-th$ interval, $[t_k, t_{k+1}]$, is thus

$$\hat{\varphi}(0) = e^{-iH_0 t_k}\tilde{\varphi}(t_k) = \varphi(t_k). \quad \text{(B.7)}$$

The Eq.(B.6) is solved by formal application of some ODE integration formula, and $\hat{\varphi}(\Delta T)$ is found. This is then transformed using Eqs.(B.5,B.3) to obtain the wave function of interest, $\varphi(t_k + \Delta T)$,

$$\varphi(t_{k+1}) = \varphi(t_k + \Delta T) = e^{-iH_0\Delta T}\hat{\varphi}(\Delta T). \quad \text{(B.8)}$$

A typical choice of ODE integration method is a Runge-Kutta 4^{th} order formula, Ref.[4]. After some manipulations, an application of the Runge-Kutta method introduces new quantites $Y_i', i = 1 \ldots 4$,

$$\begin{aligned}
Y_1' &= -i\, W\left[t_k, \varphi(t_k)\right], \\
Y_2' &= -i\, W\left[t_k + \tfrac{\Delta T}{2}, u_0(\tfrac{\Delta T}{2})\left(\varphi(t_k) + \tfrac{\Delta T}{2} Y_1'\right)\right], \\
Y_3' &= -i\, W\left[t_k + \tfrac{\Delta T}{2}, u_0(\tfrac{\Delta T}{2})\varphi(t_k) + \tfrac{\Delta T}{2} Y_2'\right], \\
Y_4' &= -i\, W\left[t_k + \Delta T, u_0(\tfrac{\Delta T}{2})\left(u_0(\tfrac{\Delta T}{2})\varphi(t_k) + \Delta T Y_3'\right)\right].
\end{aligned} \tag{B.9}$$

The final result is so-called DS-formula

$$\varphi(t_k + \Delta T) = u_0(\Delta T)\left(\varphi(t_k) + \tfrac{\Delta T}{6} Y_1'\right) + \tfrac{\Delta T}{3} u_0(\tfrac{\Delta T}{2})\left(Y_2' + Y_3'\right) + \tfrac{\Delta T}{6} Y_4'. \tag{B.10}$$

Its order of error depends on the way the operator $u_0(\tau) = \exp\left(-iH_0\tau\right)$ is approximated in the calculations. Two most common choices are

(1) Cayley approximation, with the finite difference approximation, which leads to

$$u_o(\tau) = \left(1 + \frac{i\tau}{2} H_0\right)^{-1}\left(1 - \frac{i\tau}{2} H_0\right) \tag{B.11}$$

yielding, so called, *DS2-formula*. Here, a certain caution needs to be exercised if the calculation is performed in more then one spatial dimension. Then, if the trapping potential is not symmetric (cylindrically in $2-D$, spherically in $3-D$) the corresponding coordinate pieces of H_0 do not commute if written in terms of finite differences. Thus, the choice of $H_0 = -\frac{1}{2}\nabla^2$ is imposed in order to preserve their commutativity.

(2) a combination of Fourier Transform and its inverse, which forces $H_0 = -\frac{1}{2}\nabla^2$, as well. This yields the fourth order accuracy in time, and is thus called *DS4-formula*.

In Ref.[1], the method was suggested for a nonlinear Schrödinger equation and the systems thereof, typically occuring in the theory of Bose-Einstein Condensation. There, one of the most common version of the operator W was

$$W[t, \varphi] = V_\omega \varphi + 4\pi a |\varphi|^2 \varphi, \tag{B.12}$$

where V_ω is a trapping potential. Furthermore, the $DS-$method can be easily generalized to the situation with multiple interacting fields, as demonstrated in Ref[1]. In our research we used it succesfully to solve the system of equations for coupled atom-molecule BEC, where

$$\begin{aligned} W_\varphi[t, \varphi, \psi] &= V_{\omega,\varphi}\varphi - K\varphi^* \ \psi, \\ W_\psi[t, \varphi] &= V_{\omega,\psi} - K\varphi^2, \end{aligned} \tag{B.13}$$

with $V_{\omega,\varphi}$ and $V_{\omega,\psi}$ the trapping potentials for atoms and molecules, respectively.