1. Absorbing boundaries: Exterior Complex Scaling versus Perfectly Matched Layers
2. Dephasing in coherently split Quasicondensates

Hans Peter Stimming[†]

[†] Wolfgang Pauli Institut c/o Fak. Mathematik Univ. Wien

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Part I: Exterior Complex Scaling versus Perfectly Matched Layers

Armin Scrinzi, Arnold Sommerfeld Center, LMU Munich
Norbert Mauser, WPI and Univ. Vienna

Problem: Confined simulation of infinite problem

- Computational domain is finite
- Treatment of boundary: In time dependent problem, need absorption of "outgoing parts"
  (Cases without confinement)

Absorbing boundaries in time dependent problems

Methods for boundary treatment:

- Exterior Complex Scaling (ECS): uses variable rescaling
- Perfectly Matched Layers (PML): similar to ECS
- Complex Absorbing potentials (CAP): "Optical potential", simple method, large errors
- Transparent Boundary Conditions: by Dirichlet-to-Neumann maps, most exact method

Goal: discuss theoretical differences of the ECS and PML approach, and applicability and limitations of both methods

Time dependent evolution problems

We consider time evolution problems of the type

$$i\frac{\partial}{\partial t}\psi = \mathbf{D}\psi$$

with self-adjoint operator $\mathbf{D}$.
This includes both hyperbolic and dispersive problems, 2 example cases:
1) TDSE:

$$i\frac{\partial}{\partial t}\Psi(x,t) = [-\frac{1}{2}\Delta + V(x)]\Psi(x,t)$$

2) Scalar wave equation

$$\frac{\partial^2}{\partial t^2}u = b\nabla\cdot(a\nabla u)$$

Self-adjoint case (a=b): write as system

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 & a\nabla\cdot \\ a\nabla\cdot & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}$$

and rotate coordinates $\phi_\pm = (u \pm v)/\sqrt{2}$ to get:

$$i\frac{\partial}{\partial t}\phi_\pm = \pm ia\nabla\phi_\pm$$

Absorbing boundaries by coordinate scaling

-) Exterior Complex Scaling: Introduced in the 60s for Schrödinger equations, B. Simon: see Reed - Simon Vol. IV.
-) Perfectly Matched Layers: introduced in '94 for Wave and Maxwell equations:
J. Berenger, J. Comp. Phys. **114** (2) (1994) 363-379.

F: bounded computational domain (region of interest)

Assume that the spectral functions are plane waves $|\omega\rangle = e^{i\mathbf{k}\cdot\mathbf{x}}$. Then a damping term $s(\mathbf{k},\mathbf{x})$ is added:

$$|\omega\rangle_s := e^{i\mathbf{k}\cdot\mathbf{x}(1+is(\mathbf{k},\mathbf{x}))} = e^{i\mathbf{k}\cdot\mathbf{x}} e^{-(\mathbf{k}\cdot\mathbf{x})s(\mathbf{k},\mathbf{x})}$$

such that $s(\mathbf{k},\mathbf{x}) = 0$ for $x \in F$. For

$$\mathrm{sign}(\mathbf{k}\cdot\mathbf{x}) = \mathrm{sign}[s(\mathbf{k},\mathbf{x})],$$

the re-scaled spectral functions are decaying.

Absorbing boundaries by coordinate scaling

Idea of both: rescale both the variable *and* the operator $\mathbf{D} \rightarrow \mathbf{D_s}$ such that

- its spectral functions decay and become integrable (Absorption)
- eigenvalues become complex and the time evolution is non-growing
- the solution remains unchanged inside F

Numerical algorithm:
- Cut-Off in decaying region outside of F (Boundary layer), error can be made small because of decay.

- Alternative: "Infinite Range ECS (irECS)": FEM on F, decaying element functions with infinite range outside of F.

A. Scrinzi, Phys Rev A 81, 053845 (2010)

Absorbing boundaries by complex coordinate stretching

Theoretical steps toward this goal:

(a) Introduce *real stretching* of coordinates, depending on a parameter λ, ideally show analyticity properties of the spectral representation of the operator w.r.t. λ.

(b) Analytic continuation of this scaling for *complex* $\lambda = \phi + i\theta$, such that the analytically continued spectral functions are square-integrable.

(c) Show that the eigenvalues lead to non-growing solutions

(d) Show that analyticity carries over to the solutions on F when propagated in time and solution remains unchanged on F.

Both methods follow this approach. The difference lies in the choice of λ.
For Schrödinger, ECS theory identifies a class of potentials which ensure analyticity in (a).
Also, it has been shown that some isolated EV are conserved and the cont. spectrum is rotated into the complex plane*.

* Combes, Duclos, Seiler et.al., Comm. Math. Phys. 110 (1987)

Real stretching

(a) *Real stretching:*
define a coordinate transform $x = x(y)$. Rescale both coordinate and eigenfunctions

$$|\phi\rangle \to |\phi_s\rangle := U|\phi\rangle = \sqrt{J(y)}\phi(x(y)).$$

where $J(y) = \frac{\partial x}{\partial y}$: rescaling is L^2-unitary. Now also rescale the operator, such that the rescaled equation has same form as the unstretched one:

$$i\frac{\partial}{\partial t}|\phi_s\rangle = U\mathbf{D}U^\dagger|\phi_s\rangle := \mathbf{D}_s|\phi_s\rangle \tag{1}$$

Define the stretching with $\lambda \in \mathbb{R}$ by:

$$y(x) = \int_0^x d\xi[1 + \lambda\sigma(\xi)]$$

for $\sigma \geq 0$, non-decreasing.
If the eigenfct. and ω_λ are analytic w.r.t λ, then the solution of (1) is an analytic function of λ.

Real stretching, Continuation to complex case

Example: Global scaling, one-way wave equation: $\mathbf{D} = i\partial_x$, $\sigma(\xi) \equiv 1$. Then

$$|\omega\rangle_\lambda = e^{-i\omega(1+\lambda)x}$$

The new eigenvalues are $\omega_\lambda = (1+\lambda)\omega$. Analyticity is true. When the time evolution in spectral expansion is formulated in the measure $\mu(\omega, \lambda) = \omega_\lambda$, also the propagation is analytic.

(b) *Continuation to complex plane*: let $\lambda \in \mathbb{C}$.
Need: $\mu(\omega, \lambda) = \omega_\lambda$ has negative imaginary part in order to have decay property.
Problem: sign of $\Im\{\mu\}$ depends on sign of ω, so decay can not be achieved for all ω: If $\omega < 0$, decay is true if $\Im\{\lambda\} > 0$, and vice-versa for $\omega > 0$: time evolution will be unstable !

ECS vs. PML

Remark: In case of Schrödinger equation, this problem does not appear: spectrum of $\mathbf{D} = -\Delta$ is the positive half axis, so $\Im\{\lambda\} < 0$ will give decay.

Different Approach: Perfectly Matched Layers (**PML**):
make λ dependent on eigenvalue ω: $\lambda_s = \lambda_s(\omega)$. Usual choice: $\lambda_s = \lambda/\omega$.
In the example, take:

$$\mu(\omega, \lambda) = (1 + \frac{\lambda}{\omega})\omega = \omega + \lambda$$

Then: $\Im\{\mu\} = \Im\{\lambda\}$, and decay is guaranteed for $\Im\{\lambda\} < 0$.
$->$ step (c) satisfied.

Time propagation in PML

(d), accuracy of time propagation inside of F:
need to formulate time propagation in ω-dependent scaling.
Assume completeness and orthogonality for rescaled basis, but not unitarity.
The decomposition of unity in this rescaled basis is

$$\mathbf{1} = \int_{\sigma(\mathbf{D})} |\omega, \lambda\rangle \rho(\omega, \lambda) \langle \omega, \lambda|$$

.
The time evolution in this basis is:

$$i\frac{\partial}{\partial t}\langle \omega, \lambda|\phi_\lambda(t)\rangle = \int d\omega' \langle \omega, \lambda|\mathbf{D}_\lambda|\omega', \lambda\rangle \rho(\omega', \lambda)\langle \omega', \lambda|\phi_\lambda(t)\rangle$$

Time propagation in PML

Let us assume $\mathbf{D}_\lambda$ is defined such that

$$\langle \omega, \lambda | \mathbf{D}_\lambda | \omega', \lambda \rangle = \delta(\omega - \omega') g(\omega, \lambda),$$

then

$$i \frac{\partial}{\partial t} \langle \omega, \lambda | \phi_\lambda(t) \rangle = g(\omega, \lambda) \rho(\omega, \lambda) \langle \omega, \lambda | \phi_\lambda(t) \rangle$$

with the solutions

$$\langle \omega, \lambda | \phi_\lambda(t) \rangle = \exp[-itg(\omega, \lambda)\rho(\omega, \lambda)] \langle \omega, \lambda | \phi_\lambda(0) \rangle.$$

In x-space, write the basis functions as

$$\langle x | \omega, \lambda \rangle =: \kappa_\omega(x, \lambda) = \kappa_\omega(x, 0) \quad \forall x \in F,$$

define $\tilde{\phi}_\lambda(\omega, 0) \langle \omega, \lambda | \phi_\lambda(0) \rangle$, and the solution in x-space is

$$\phi_\lambda(x, t) = \int d\omega \kappa_\omega(x, \lambda) \rho(\omega, \lambda) e^{-itg(\omega, \lambda)\rho(\omega, \lambda)} \tilde{\phi}_\lambda(\omega, 0).$$

Time propagation in PML

The time propagation is accurate if

$$\phi_\lambda(x,t) = \phi_0(x,t) \quad \forall x \in F$$

under the condition that the initial data is constrained to F. By assumption, on F the $\kappa_\omega(x,\lambda)$ do not depend on λ, i.e.

$$\phi_\lambda(x,t) = \int d\omega \kappa_\omega(x) \rho(\omega,\lambda) e^{-itg(\omega,\lambda)\rho(\omega,\lambda)} \tilde{\phi}(\omega,0)$$

for $x \in F$. Compare this to the solution according to the original time-evolution:

$$\phi(x,t) = \int d\omega \kappa_\omega(x) e^{-it\omega} \tilde{\phi}(\omega,0).$$

• For ECS with ω-independent scaling: $\rho \equiv 1$ and $g(\omega,\lambda) = \omega$, so time evolution is exact

Time propagation in PML

• For the case of PML:
-) $\rho(\omega, \lambda)$ can be absorbed in the initial data $\tilde{\phi}_\lambda(\omega, 0)$.
-) need moreover that $g(\omega, \lambda)\rho(\omega, \lambda) = \omega$: need to define $\mathbf{D}_\lambda$ in such a way that $g(\omega, \lambda) = \frac{\omega}{\rho(\omega, \lambda)}$. In general, this leads to an integro-differential operator.

In usual applications of PML: no unitary rescaling of solution.
Additional ω-dependence is treated in time domain by a set of auxillary equations outside of F.
The solutions do not always decay in time.

Time propagation for PML and ECS

Example for failure of PML: Coaxial waveguides (Aniosotropic case).
Different signs of phase velocity and group velocity: at same phase velocity, there exist solutions with both signs of group velocity: "Backward Waves".
PML leads to instabilities.

Ibanescu, Johnson et.al., PRL 92, 063903 (2004),
Loh, Oskooi, Johnson et.al., Phys. Rev. E 79, 065601(R) (2009)

Exterior Complex Scaling versus Perfectly Matched Layers

Conclusion:

- PML and ECS are two different methods to obtain absorption by scaling.
- ECS works well for Schrödinger type equations: decay guaranteed, analyticity for many applications (depending on potential)
- For hyperbolic equations, ECS fails.
- PML results in reflectionless absorption. Treatment of hyperbolic eqations possible.
- Time evolution of PML can be distorted, stability is not always guaranteed.

Part II: Dephasing in coherently split Quasicondensate

Collaboration:
J. Schmiedmayer, Atom Institut, Vienna Tech. Univ.
I. Mazets, Atom Institut, Vienna Tech. Univ.
Norbert Mauser, WPI and Univ. Vienna

- Experiment: Splitting of BEC in double well trap
- (small) fluctuations exist in phase and density: Quasicondensate
- Decay of correlation after splitting

Experiment: Matter-wave interference in a double well

Analogous to the double-slit experiment for photons (light),
but now for atoms (rubidium) of a Bose-Einstein condensate (BEC)

- Creation of BEC at extremely low temperatures ($\sim 10\mu$K), sophisticated cooling techniques necessary
- BEC confined in a trap: harmonic potential well, realized with combination of static and radio-frequency (RF) magnetic fields, numerical simulation starts here
- Splitting the condensate: splitting single well $\rightarrow$ double well by slowly changing parameters of RF-currents
- Free expansion: Sudden switch off of the external potential, recombine BEC clouds in time-of-flight expansion
- Measurement of interference pattern, ...

Dephasing in coherently split Quasicondensates

Fluctuations are completely correlated at moment of splitting, but during time evolution, correlation decays.
Model this case by two GPE equations in $1-d$: $\psi_1(z,t)$, $\psi_2(z,t)$.
- Fluctuations in initial data modeled as thermal excitations
- Coherent fluctuations in two condensates modeled by excitations in odd and even modes
Let $\psi_j(z,0) = n_j(z,0)e^{i\phi_j(z,0)}$, and

$$\begin{aligned} \phi_{1,2}(z,0) &= \frac{\phi_+(z,0) \pm \phi_-(z,0)}{\sqrt{2}}, \\ n_{1,2}(z,0) &= n_{1\mathrm{D}} + \frac{\delta n_+(z,0) \pm \delta n_-(z,0)}{\sqrt{2}} \end{aligned}$$

where

$$\begin{aligned} \delta n_\pm(z,0) &= 2\sqrt{\frac{n_{1\mathrm{D}}}{L}} \sum_k \sqrt{S_k} B_k^\pm \cos(kz + \zeta_k^\pm), \\ \phi_\pm(z,0) &= \frac{1}{\sqrt{n_{1\mathrm{D}} L}} \sum_k \frac{1}{\sqrt{S_k}} B_k^\pm \sin(kz + \zeta_k^\pm), \end{aligned}$$

where $B_k^\pm$ is a positive random number whose square is exponentially distributed with mean

$$\langle |B_k^\pm|^2 \rangle = \frac{k_{\mathrm{B}} T_\pm}{\sqrt{\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2\mu\right)}},$$

Dephasing in coherently split Quasicondensates

Parameters in this model:
n_{1D}: condensate background density, T: temperature ,
ω_r: radial trapping frequency for quasi-1D trap

Chemical potential: $\mu = 2\hbar\omega_r n_{1D} a_s$.
Coherence factor (Quantity of interest):

$$\Psi(t) = \langle\ \psi_1^*(z,t)\psi_2(z,t)\ \rangle$$

Dephasing:

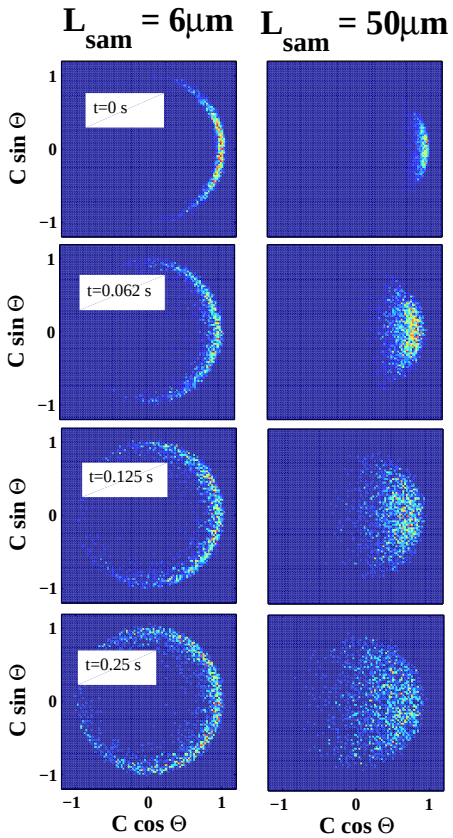
- propagate GPE in time
- evaluate correlation $\int \psi_1^*(z,t)\psi_2(z,t)dz$
- obtain $\Psi(t)$ by averaging over all statistical realizations

Theory (and experiment) : $\Psi(t) \sim \exp\left[-\left(\frac{t}{t_0}\right)^{\alpha}\right], \quad \alpha = 2/3,\ t_0 = ?$

Theoretical hypothesis: $t_0 \sim \frac{n_{1D}^2}{T^2}$, independent of ω_r.

Dephasing in coherently split Quasicondensates

Simulation results: Time evolution of the full distribution function



Dephasing in coherently split Quasicondensates

Simulation results:

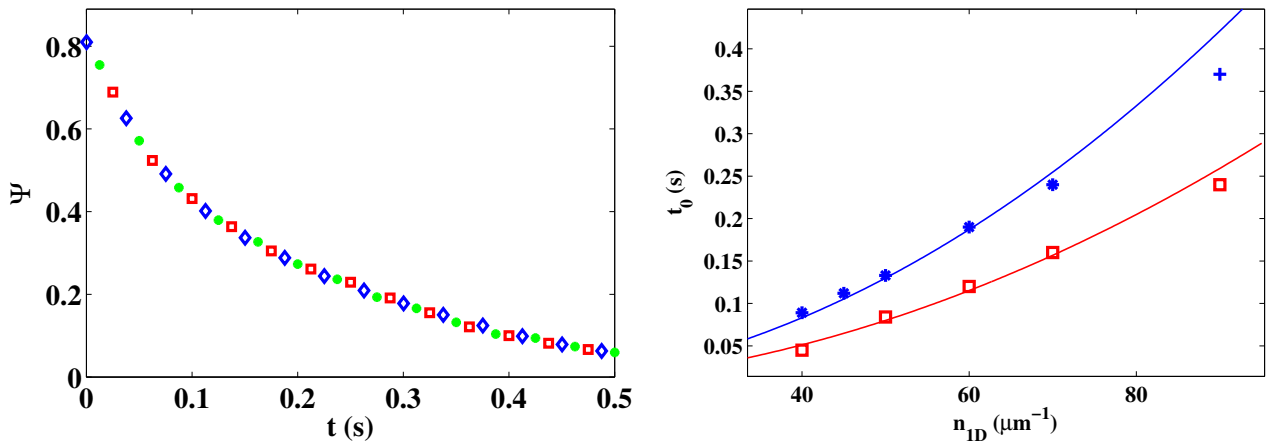


Figure: Left: coherence factor $\Psi(t)$ for different radial trapping frequencies, right: Dependence of t_0 on n_{1D}, for $T_+ = 70$ nK and 90 nK.

Dephasing in coherently split Quasicondensates

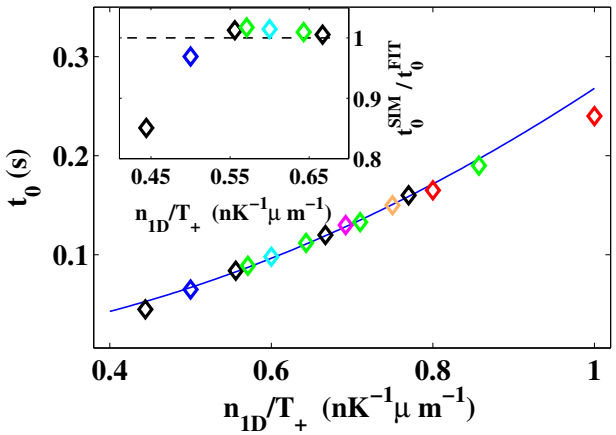


Figure: Dependence of relaxation time t_0 on n_{1D}/T

"Fluctuations and stochastic processes in one-dimensional many-body quantum systems", H.P. Stimming, N.J. Mauser, J. Schmiedmayer, I.E. Mazets, Phys.Rev.Lett **105** (2010) 015301

"Dephasing in coherently-split quasicondensates", H.P. Stimming, N.J. Mauser, J. Schmiedmayer, I.E. Mazets, Phys.Rev.A **63** (2011) 023618

Thank you for your attention.