Asymptotic preserving schemes for quantum kinetic equations

Lorenzo Pareschi

Department of Mathematics and Computer Science
University of Ferrara, Italy

http://www.lorenzopareschi.com

Joint research with:
Giacomo Dimarco (University of Toulouse, France)

Quantum systems: a mathematical journey form few to many particles
(CSCAMM, may 13-16 2013)

Outline

1. Introduction
2. Quantum kinetic theory
   - The quantum Boltzmann equation (QBE)
   - Equilibrium states
   - Ergodic approximation
3. Numerical methods
   - The Implicit-Explicit (IMEX) paradigm
   - IMEX-RK for the Boltzmann equation
   - Discretization of the collision operator
   - Numerical tests
4. Summary and future research

Motivations

- The computation of *fluid-kinetic interfaces* and *asymptotic behaviors* involves multiple scales where most numerical methods lose their efficiency because they are forced to operate on a very short time scale.
- *Asymptotic-preserving* (*AP*) schemes represent a powerful tool for the numerical treatment of such problems. A suitable combination of implicit and explicit treatment of the stiff terms permits to achieve the desired asymptotic properties at the cost of an explicit scheme.
- Similar techniques can be adopted when dealing with kinetic equation of *Boltzmann-type*. Here, however, the major challenge is represented by the complicated nonlinear structure of the collisional operator which makes prohibitively expensive the use of implicit solvers for the stiff collision term.
- Additional difficulties are given by the need to preserve some relevant *physical properties* like conservation of mass, momentum and energy, nonnegativity of the solution, entropy inequality, steady states, ...

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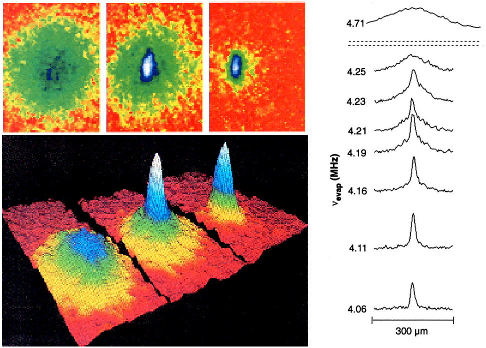
Bose-Einstein condensation: experimental evidence

2001 Nobel Prize in Physics (A.Cornell, W.Ketterle,C.Wiemann)



Momentum density of BEC in rubidium (Science 1995, Anderson, Ensher, Matthews, Wiemann, Cornell).

A large fraction of Bosons occupies the lowest energy quantum state. Predicted by S.Bose, A.Einstein '24.

Outline

The quantum Boltzmann equation (QBE)[1]

Gas of interacting particles, which are trapped by a confining potential $V = V(x)$ (with $\min V(x) = 0$). Let $F = F(p, x, t) \geq 0$ be the phase-space density of particles with momentum p and position x.

The quantum Boltzmann equation (QBE)

$$\frac{\partial F}{\partial t} + p \cdot \nabla_x F - \nabla_x V(x) \cdot \nabla_p F = \frac{1}{\tau} Q(F, F), \quad t > 0,$$

where $\tau > 0$ is the Knudsen number.

$$Q(F,F)(p,x,t) = \int_{\mathbb{R}^9} \delta(p + p_* - p' - p'_*)\, \delta\left(\frac{|p|^2}{2} + \frac{|p_*|^2}{2} - \frac{|p'|^2}{2} - \frac{|p'_*|^2}{2}\right) w(p, p_*, p', p'_*) C(F)\, dp_*\, dp'\, dp'_*,$$

with $C(F) = F'F'_*(1 + \vartheta F)(1 + \vartheta F_*) - FF_*(1 + \vartheta F')(1 + \vartheta F'_*)$ and $F = F(p, x, t)$, $F_* = F(p_*, x, t)$, $F' = F(p', x, t)$, $F'_* = F(p'_*, x, t)$.

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The quantum collision operator

The function $w \geq 0$ is related to the differential cross section.

The QBE includes (namely for $\vartheta = 0$) the classical equation of the Maxwell-Boltzmann statistics as a special case. It differs from the latter in the case of Bose-Einstein statistics ($\vartheta = +1$) and in the case of Fermi-Dirac statistics ($\vartheta = -1$).

The collision operator can be written in the conventional form as

$$Q(F,F)(p,x,t) \quad = \quad 2\int_{\mathbb{R}^3\times S^2} |p-p_*|\tilde{w}(p,p_*,|p-p_*|n,p+p_*)C(F)\,dp_*\,d\sigma,$$

where

$$\tilde{w}(p,p_*,|p-p_*|\sigma,p+p_*) = w(p,p_*,p',p'_*), \quad \sigma = (p-p_*)/|p-p_*|$$

$$p' = \frac{1}{2}(p+p_*+|p-p_*|\sigma), \quad p'_* = \frac{1}{2}(p+p_*-|p-p_*|\sigma).$$

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Physical properties

Let $\phi = \phi(p)$ be a test function. From the symmetries of w we have

$$\int_{\mathbb{R}^3} Q(F,F)\phi\,dp = \frac{1}{4}\int_{\mathbb{R}^{12}} \delta(p+p_* - p' - p'_*)\,\delta\left(\frac{|p|^2}{2}+\frac{|p_*|^2}{2}-\frac{|p'|^2}{2}-\frac{|p'_*|^2}{2}\right) w(p,p_*,p',p'_*)C(F)(\phi+\phi_*-\phi'-\phi'_*)\,dp\,dp_*\,dp'\,dp'_*,$$

Taking $\phi = 1$, $\phi = p$ and $\phi = |p|^2$ we obtain the particle number, momentum and energy conservations

$$\int_{\mathbb{R}^3} Q(F,F)\begin{pmatrix}1\\ p\\ |p|^2\end{pmatrix} dp = 0.$$

Taking $\phi = \ln(1+\vartheta F) - \ln(F)$ we have the entropy inequality

$$\int_{\mathbb{R}^3} Q(F,F)(\ln(1+\vartheta F) - \ln(F))\,dp \geq 0.$$

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Equilibrium states

In the homogeneous case, $V(x) = 0$ and F independent of x conservations and increasing of entropy imply that an equilibrium state, i.e. a function $F_\infty \geq 0$ such that $Q(F_\infty, F_\infty) = 0$, realizes the maximum of the entropy under the moments constraint

$$\int_{\mathbb{R}^3} F_\infty(p) \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp = \begin{pmatrix} M_\infty \\ P_\infty \\ E_\infty \end{pmatrix}.$$

The equilibrium states have the form

$$F_\infty(p) = \frac{1}{\exp(a|p|^2/2 - b \cdot p - c) - \vartheta},$$

with $a, c \in \mathbb{R}$ and $b \in \mathbb{R}^3$. The function is called a Maxwellian when $\vartheta = 0$, a Bose-Einstein when $\vartheta > 0$ and a Fermi-Dirac when $\vartheta < 0$.
Note that, except for $\vartheta = 0$, given $M_\infty > 0$, $P_\infty \in \mathbb{R}^3$ and $E_\infty > 0$ it is not always possible to compute a, b and c such that $F_\infty \geq 0$.

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Equilibrium states II

- In the case $\vartheta > 0$ it was first observed by Bose and Einstein[2] that the set of steady distributions has to include a Dirac mass. For any $M_\infty > 0$, $P_\infty \in \mathbb{R}^3$ and $E_\infty > 0$ there exist a generalized Bose-Einstein distribution of the form[3]

$$F_\infty(p) = \frac{1}{\exp(\alpha|p-P|^2+\beta_+)-\vartheta} - \beta_-\delta(p),$$

with $\alpha, \beta \in \mathbb{R}$, $\beta_+ = \max(\beta, 0)$ and $\beta_- = -\max(-\beta, 0)$.

- In the case $\vartheta < 0$ we have the additional constraint $0 \le F_\infty(p) \le \vartheta$ and we have to introduce the saturated Fermi-Dirac state. Taking $\vartheta = -1$, for any $M_\infty > 0$, $P_\infty \in \mathbb{R}^3$ and $E_\infty > 0$ satisfying $5E_\infty \ge (4\pi)^{2/3}(3M_\infty)^{5/3}$ there exist a Fermi-Dirac distribution (saturated or not) defined as[3]

$$F_\infty(p) = \begin{cases} \dfrac{1}{\exp(\alpha|p-P|^2+\beta)+1}, & 5E_\infty > (4\pi)^{2/3}(3M_\infty)^{5/3}, \\ \chi(|p-P| \le C), & 5E_\infty = (4\pi)^{2/3}(3M_\infty)^{5/3}, \end{cases}$$

with $\alpha, \beta \in \mathbb{R}$, $\chi(I)$ the indicator function of the set I and $C > 0$.

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[3] X.Lu '00, M.Escobedo, S.Mischler, M.A.Valle '03

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Numerical requirements

Our purpose is to derive efficient time integration methods for the QBE, which maintain the basic analytical and physical features of the continuous problem, namely

- Asymptotic-preservation as $\tau \to 0$
- Conservations
- Entropy growth
- Equilibrium distributions (even in the challenging concentration/saturation cases)

In addition, from a numerical point of view it is also essential to deal with

- Accuracy
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Ergodic approximation

The ergodic approximation assumes a particle distribution which only depends on the total energy $H(x,p) = \frac{|p|^2}{2} + V(x)$, thus $F(x,p,t) = f(H(x,p),t)$, where $f(\cdot,t) \geq 0$ is the particle density in energy space.

Mathematically we approximate the whole QBE using the projection operator[4]

$$\mathcal{P}(g(x,p,t))(\varepsilon) = \int_{\mathbb{R}^6} g(x,p,t)\delta\left(\varepsilon - H(x,p)\right) dp\, dx, \qquad \forall\, g.$$

Ergodic QBE

$$\rho(\varepsilon)\frac{\partial f(\varepsilon)}{\partial t} = \frac{1}{\tau}\int_{\mathbb{R}^3_+} S(\varepsilon,\varepsilon_*,\varepsilon',\varepsilon'_*)[f'_*(1+\vartheta f)(1+\vartheta f_*)-f f_*(1+\vartheta f')(1+\vartheta f'_*)]d\varepsilon_*\, d\varepsilon'\, d\varepsilon'_*$$

$$\rho(\varepsilon) = \int_{\mathbb{R}^6} \delta\left(\varepsilon - H(x,p)\right) dp\, dx = 4\pi \int_{V(x)<\varepsilon} \sqrt{2(\varepsilon - V(x))}\, dx.$$

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Ergodic approximation II

Taking $w \equiv 1$ and setting $\varepsilon_{\min} = \min\{\varepsilon, \varepsilon_*, \varepsilon', \varepsilon'_*\}$ we have

$$S(\varepsilon, \varepsilon_*, \varepsilon', \varepsilon'_*) = 4\pi^2 \delta\left(\varepsilon + \varepsilon_* - \varepsilon' - \varepsilon'_*\right) \rho(\varepsilon_{\min}).$$

In a space homogeneous setting, $V(x) \equiv 0$ and F independent of x we have

$$\rho(\varepsilon) = \int_{\mathbb{R}^3} \delta\left(\varepsilon - \frac{|p|^2}{2}\right) dp = 4\pi\sqrt{2\varepsilon}.$$

Similarly for a harmonic potential $V(x) = |x|^2/2$ we obtain $\rho(\varepsilon) = \varepsilon^2/2$.

Density and energy (momentum vanishes) can be recovered

$$n(x,t) = 4\pi \int_{V(x)}^{\infty} f(\varepsilon,t)\sqrt{2(\varepsilon - V(x))}\,d\varepsilon,$$

$$e(x,t) = 4\pi \int_{V(x)}^{\infty} f(\varepsilon,t)(2(\varepsilon - V(x)))^{3/2}\,d\varepsilon.$$

Moreover the total mass and energy are given by

$$M(t) = \int_{\mathbb{R}_+} f(\varepsilon,t)\rho(\varepsilon)\,d\varepsilon, \quad E(t) = \int_{\mathbb{R}_+} f(\varepsilon,t)\rho(\varepsilon)\varepsilon\,d\varepsilon.$$

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Physical properties

Let $\phi = \phi(\varepsilon)$ be a test function. Then using the symmetries of S we have

$$\begin{aligned}\int_0^\infty Q(f)\phi d\varepsilon &= \frac{1}{4}\int_{\mathbb{R}_+^4} \delta(\varepsilon+\varepsilon_*-\varepsilon'-\varepsilon'_*)S(\varepsilon,\varepsilon_*,\varepsilon',\varepsilon'_*)[f'f'_*(1+\vartheta f)(1+\vartheta f_*)\\ &- ff_*(1+\vartheta f')(1+\vartheta f'_*)][\phi+\phi_*-\phi'-\phi'_*]d\varepsilon d\varepsilon_* d\varepsilon' d\varepsilon'_*.\end{aligned}$$

As a consequence we have the following collision invariants

$$\phi(\varepsilon)\equiv 1 \quad \Rightarrow \quad \int_0^\infty Q(f)(\varepsilon)\,d\varepsilon = 0,$$

$$\phi(\varepsilon)\equiv \varepsilon \quad \Rightarrow \quad \int_0^\infty Q(f)(\varepsilon)\varepsilon\,d\varepsilon = 0.$$

Similarly the H-theorem is derived taking $\phi(\varepsilon) = \ln(1+\vartheta f(\varepsilon)) - \ln f(\varepsilon)$

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Equilibrium states I

Again in the case of bosons, $\vartheta > 0$, the class of 'regular' Bose-Einstein distributions is not sufficient to assume all possible values of equilibrium mass and energy M_∞, E_∞ such that Dirac distribution have to be added. More precisely, for every pair $(M_\infty, E_\infty) \in \mathbb{R}^2_+$ there exist $\alpha \geq 0$, $\beta \in \mathbb{R}$ such that the generalized Bose-Einstein distribution

$$f_\infty(\varepsilon) = \frac{1}{e^{\alpha\varepsilon+\beta_+} - \vartheta} - \beta_- \delta(\varepsilon),$$

is an equilibrium state of the QBE.

A similar analysis in the case of fermions lead to the saturated Fermi-Dirac distributions. More precisely, taking $\vartheta = -1$, for any pair $(M_\infty, E_\infty) \in \mathbb{R}^2_+$ satisfying $5E_\infty \geq (4\pi)^{2/3}(3M_\infty)^{5/3}$ there exist a Fermi-Dirac distribution (saturated or not) defined as

$$f_\infty(\varepsilon) = \begin{cases} \dfrac{1}{e^{\alpha\varepsilon+\beta} + 1}, & 5E_\infty > (4\pi)^{2/3}(3M_\infty)^{5/3}, \\ \chi(\varepsilon \leq C^2/2), & 5E_\infty = (4\pi)^{2/3}(3M_\infty)^{5/3}, \end{cases}$$

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Outline

Numerical methods

Many practical application involves systems of differential equations of the form

The IMEX paradigm

$$U' = \underbrace{\mathcal{F}(U)}_{\text{non stiff term}} + \underbrace{\mathcal{G}(U)}_{\text{stiff term}},$$

where $\mathcal{F}$ and $\mathcal{G}$, eventually obtained as suitable finite-difference or finite-element approximations of spatial derivatives (*method of lines*), induce considerably different time scales.

- Although the problem is stiff as a whole, the use of fully implicit solvers originates a nonlinear system of equations involving also the non stiff term $\mathcal{F}$.
- Thus it is highly desirable to have a combination of implicit and explicit discretization terms to resolve stiff and non–stiff dynamics accordingly.
- IMEX Runge-Kutta methods[5] have been developed to deal with the numerical integration of *hyperbolic balance laws*, *kinetic equations*, *convection–diffusion equations* and *singular perturbed problems*.

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IMEX Runge-Kutta methods

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$$U_i = U^n + \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} \mathcal{F}(t_0 + \tilde{c}_j \Delta t, U_j) + \Delta t \sum_{j=1}^{\nu} a_{ij} \mathcal{G}(t_0 + c_j \Delta t, U_j),$$

$$U^{n+1} = U^n + \Delta t \sum_{i=1}^{\nu} \tilde{w}_i \mathcal{F}(t_0 + \tilde{c}_i \Delta t, U_i) + \Delta t \sum_{i=1}^{\nu} w_i \mathcal{G}(t_0 + c_i \Delta t, U_i).$$

Explicit scheme characterized by the $\nu \times \nu$ matrix $\tilde{A} = (\tilde{a}_{ij})$, $\tilde{a}_{ij} = 0$, $j \geq i$ and the coefficient vectors are $\tilde{c} = (\tilde{c}_1, \dots, \tilde{c}_\nu)^T$, $\tilde{c}_i = \sum_{j=1}^{i-1} \tilde{a}_{ij}$, $\tilde{w} = (\tilde{w}_1, \dots, \tilde{w}_\nu)^T$.
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Order conditions

- If $w_i = \tilde{w}_i$ and $c_i = \tilde{c}_i$ mixed conditions are automatically satisfied. This is not true for higher that third order accuracy
- IMEX-RK schemes are a particular case of *additive Runge-Kutta (ARK)* methods. Higher order conditions can be derived using a generalization of Butcher 1-trees to 2-trees[6].
- In addition to the order conditions, other requirements (*strong stability preserving*, *AP*, *positivity*, etc) may impose further conditions on the coefficients.
- The schemes can be schematically summarized using a *double Butcher tableu* of the type

$$\begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{w}^T \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & w^T \end{array}$$

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Remarks

- Following the above design principles it is possible to construct schemes up to *third-order* that satisfy the AP-property for any set of initial data and up to *fourth-order* for well-prepared initial data.
- Such schemes have been successfully applied to *singularly perturbed problems* and *hyperbolic relaxation system* in the zero-relaxation limit.
- The same schemes can be applied also to other limiting asymptotic behavior, like the case of *diffusion limits*, provided that the system is partitioned correctly in to stiff and non stiff components [7].
- For *kinetic equations* additional difficulties are present, due to the nonnegativity requirement and the complicated structure of the collision term whose inversion is prohibitively expensive.
- Other related approaches are based on *IMEX multistep* methods [8] and *exponential methods* [9].

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Outline

Design principles for the Boltzmann case

- The goal is to construct AP and asymptotically accurate schemes *avoiding the implicit solution* of the collision term of the Boltzmann equation.
- The main idea is to use the fact that when τ is small we do not really need to resolve the whole collision operator since we know that $f \approx f_\infty$.
- On the other hand when $f \approx f_\infty$ we know that the collision operator is well approximated by its linear counterpart $Q(f_\infty, f)$ or directly by a BGK or an improved *ES-BGK* relaxation operator.
- If we denote by $L(f)$ the selected linear approximating operator we can write [10]

$$Q(f,f) = L(f) + G(f), \quad G(f) = Q(f,f) - L(f).$$

▶ The idea now is to be implicit (or exact) in the linear part $L(f)$ and explicit in the deviations from equilibrium $G(f)$.

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IMEX-RK for the Boltzmann equation

In the sequel we assume $L(f) = \mu(f_\infty - f)$, $\mu > 0$. The IMEX-RK scheme take the form[11]

IMEX-RK for Bolztmann

$$F^{(i)} = f^n + \Delta t \sum_{j=1}^{i-1} \widetilde{a}_{ij} \frac{1}{\tau} G(F^{(j)}) + \Delta t \sum_{j=1}^{\nu} a_{ij} \frac{\mu}{\tau} (F_\infty^{(j)} - F^{(j)})$$

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AP-property

Consider now the stage i in the original IMEX scheme and solve it for $(F_\infty^{(i)} - F^{(i)})$

$$\Delta t(F_\infty^{(i)} - F^{(i)}) = \frac{\tau}{\mu}\sum_{j=1}^{i} b_{ij}\left[F^{(j)} - f^n - \frac{\Delta t}{\tau}\sum_{h=1}^{j-1}\widetilde{a}_{jh}G(F^{(h)})\right].$$

As $\tau \to 0$, if $\det(A) \neq 0$, we get

$$F^{(i)} = F_\infty^{(i)}, \quad i = 1, \ldots, \nu.$$

In fact, $\widetilde{A}$ is lower triangular with $\widetilde{a}_{ii} = 0$ and we have a hierarchy of equations such that $F^{(h)} = F_\infty^{(h)}, h = 1, .., j-1$.

Stiffly accurate schemes

However, now the last level still depends on τ. After some manipulations it reads

$$
\begin{aligned}
f^{n+1} &= f^n\left(1-\sum_{i,j} w_i b_{ij}\right)+\frac{\Delta t}{\tau}\sum_{i=1}^{\nu}\widetilde{w}_i G(F^{(i)}) \\
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Now for small values of τ the scheme turns out to be unstable since f^{n+1} is not bounded. A remedy to this fact, is to consider *stiffly accurate schemes* for which $f^{n+1}=F^{(\nu)}$ and so $f^{n+1}\to f^{n+1}_{\infty}$ as $\tau\to 0$.

- This is guaranteed if $a_{\nu i}=w_i$ and $\widetilde{a}_{\nu i}=\widetilde{w}_i$, $i=1,\dots,\nu$.
- On the contrary to standard IMEX schemes, for the penalized Boltzmann case the stiffly accurate property is mandatory to have a stable AP scheme.

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- On the contrary to standard IMEX schemes, for the penalized Boltzmann case the stiffly accurate property is mandatory to have a stable AP scheme.

Positive and entropic IMEX schemes

Theorem

A sufficient condition to guarantee the positivity of the IMEX method for the Boltzmann equation is that it is stiffly accurate and the coefficients satisfy

$$(I+zA)^{-1}e \geq 0, \quad (I+zA)^{-1}(A-\tilde{A})e \geq 0, \qquad (I+zA)^{-1}\tilde{A} \geq 0,$$

where $z = \mu \Delta t/\tau$.

Since the above theorem is based on a convexity argument it follows that the schemes are also entropic provided we have an estimate of the type [12]

$$H(Q(f,f) + \mu f) \leq H(f),$$

where $H(\cdot)$ is the entropy functional.

[12] C.Villani '98, G.Toscani, C.Villani '99

Positive and entropic IMEX schemes

Theorem

A sufficient condition to guarantee the positivity of the IMEX method for the Boltzmann equation is that it is stiffly accurate and the coefficients satisfy

$$(I + zA)^{-1}e \geq 0, \quad (I + zA)^{-1}(A - \tilde{A})e \geq 0, \qquad (I + zA)^{-1}\tilde{A} \geq 0,$$

where $z = \mu\Delta t/\tau$.

Since the above theorem is based on a convexity argument it follows that the schemes are also entropic provided we have an estimate of the type [12]

$$H(Q(f, f) + \mu f) \leq H(f),$$

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Outline

Discretization of the collision operator

Let us consider the case of bosons, $\vartheta = 1$. We introduce a set of equally spaced discrete energy grid points $\varepsilon_i,\ i = 1, \dots N$ in the energy interval $[0, R]$. The numerical method for $Q_R(f)$ takes the form[13]

$$
\begin{aligned}
Q_R(f)(\varepsilon_i) \approx \tilde{Q}_R(f)(\varepsilon_i) \quad &= \quad (\Delta\varepsilon)^3 \sum_{j,k,l=1}^{N} \delta_{ij}^{kl}\, \rho(\varepsilon_{\min})[f_k f_l (1+f_i)(1+f_j) \\
&- \quad f_i f_j (1+f_k)(1+f_l)]\chi(\varepsilon_i \leq R),
\end{aligned}
$$

where $f_i \approx f(\varepsilon_i)$ and $\varepsilon_{\min} = \min\{\varepsilon_i, \varepsilon_j, \varepsilon_k, \varepsilon_l\}$ and

$$
\delta_{ij}^{kl} = \begin{cases} 1/\Delta\varepsilon & i+j = k+l \\ 0 & \text{otherwise.} \end{cases}
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The quantities δ_{ij}^{kl} are a suitable discretization of the δ-function on the grid (which reduce the points in the sum to a discrete index set which satisfies the relation $i + j = k + l$). Taking $\varepsilon_i = (i-1)\Delta\varepsilon$ we have a first order method, whereas the choice $\varepsilon_i = (i - 1/2)\Delta\varepsilon$ originates a second order scheme.

[13] P.Markowich, L.Pareschi, 2005 - W.Bao, P.Markowich, L.Pareschi, 2004

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Properties

We consider the set of ODEs which originates from this discretization

$$\rho(\varepsilon_i)\frac{df_i}{dt} = \frac{1}{\tau}\tilde{Q}_R(f)(\varepsilon_i), \quad t > 0, \tag{1}$$

$$f_i(t=0) = f_{0,R}(\varepsilon_i) \geq 0. \tag{2}$$

Proposition 1

The solutions of (1), (2) satisfy the following conservation properties and H-theorem

$$\Delta\varepsilon \sum_{i=1}^{N} \rho(\varepsilon_i)\frac{df_i}{dt}\phi(\varepsilon_i) = 0, \qquad \phi(\varepsilon) = 1, \quad \phi(\varepsilon) = \varepsilon,$$

$$\Delta\varepsilon \sum_{i=1}^{N} \rho(\varepsilon_i)\frac{dh(f_i)}{dt} \geq 0, \qquad h(f_i) = (1+f_i)\ln(1+f_i) - f_i \ln f_i.$$

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Discrete steady states

From the above theorem we can show that the scheme admits regular Bose-Einstein equilibrium of the form

$$f_\infty(\varepsilon_i) = \frac{1}{e^{\tilde{\alpha}\varepsilon_i + \tilde{\beta}} - 1}, \qquad \tilde{\alpha}, \tilde{\beta} > 0,$$

where the values $\tilde{\alpha}, \tilde{\beta}$ are computed by solving, for a given mass-energy pair (M_∞, E_∞), the nonlinear system

$$\begin{aligned} \Delta\varepsilon \sum_{i=1}^{N} \rho(\varepsilon_i) f_\infty(\varepsilon_i) &= M_\infty, \\ \Delta\varepsilon \sum_{i=1}^{N} \rho(\varepsilon_i) \varepsilon_i f_\infty(\varepsilon_i) &= E_\infty. \end{aligned}$$

If the above system cannot be solved for positive $\tilde{\alpha}$ and $\tilde{\beta}$ then condensation occurs. Note however that for the second order method, since the value $\varepsilon = 0$ is not present in the scheme, we do not expect blow-up of the numerical solution but the formation of a discrete Dirac delta at $\varepsilon_1 = \Delta\varepsilon/2$ of the form $1/\Delta\varepsilon$.

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Fast algorithms

The evaluation of the double sum in $\tilde{Q}_R(f)(\varepsilon_i)$ at the point ε_i requires $(2(i-1)(N-i+1)+N^2)/2$ operations. The overall cost for all N points is then approximately $2N^3/3$.

- Using *transform techniques* based on FFT and a domain decomposition the $O(N^3)$ cost can be reduced to $O(N^2 \log_2 N)$ [14].
- Recently using a more refined decomposition the overall cost has been reduced to quasi optimal value $O(N(\log_2 N)^2)$ [15].
- In the general non ergodic case the *fast spectral method* developed by Pareschi and Mouhot can be adapted to the QBE, fast algorithms have been developed but due to the cubic nonlinearity they are less efficient compared to the case $\theta = 0$ [16].

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Outline

1. Introduction
2. Quantum kinetic theory
   - The quantum Boltzmann equation (QBE)
   - Equilibrium states
   - Ergodic approximation
3. Numerical methods
   - The Implicit-Explicit (IMEX) paradigm
   - IMEX-RK for the Boltzmann equation
   - Discretization of the collision operator
   - Numerical tests
4. Summary and future research

Numerical tests and applications

The time integration is performed with different IMEX Runge-Kutta schemes of second and third order after dividing the semidiscrete schemes by $\rho(\varepsilon_i)$ and thus rewriting

$$\begin{aligned}\frac{\partial f_i}{\partial t} &= \frac{(\Delta\varepsilon)^2}{\tau} \sum_{\substack{j,l=1 \\ 1\le k=i+j-l\le N}}^{N} \frac{\rho(\varepsilon_{\min})}{\rho(\varepsilon_i)}[f_k f_l(1+f_i)(1+f_j) \\ &- f_i f_j(1+f_k)(1+f_l)].\end{aligned}$$

In all our numerical tests the density of states is given by $\rho(\varepsilon) = \varepsilon^2/2,$ which corresponds to an harmonic potential.

Note that $0 \le \rho(\varepsilon_{\min})/\rho(\varepsilon_i) \le 1$ for $\varepsilon_i \neq 0$ and that as $\varepsilon_i \to 0$ we have $\rho(\varepsilon_{\min})/\rho(\varepsilon_i) \to 1$.

Standard stability condition of an explicit scheme is $\Delta t \le \tau/L(f)$ where

$$L(f) = (\Delta\varepsilon)^2 \sum_{\substack{j,l=1 \\ 1\le k=i+j-l\le N}}^{N} f_j(1+f_k)(1+f_l).$$

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Accuracy analysis and steady states

- The first test case has been used to check the numerical convergence of our time discretization methods by neglecting the energy discretization error (this is achieved using the second order method and very small mesh sizes).
- The initial datum is a Gaussian profile centered at $R/2$

$$f = \exp(-4(\varepsilon - R/2)^2),$$

with $R = 10$. The final integration time is $T = 4.0$. We report the convergence rates in the L_1-norm obtained with the different schemes for different $\tau = 1, 0.1, 0.01$. In this case the mass-energy pair is subcritical.

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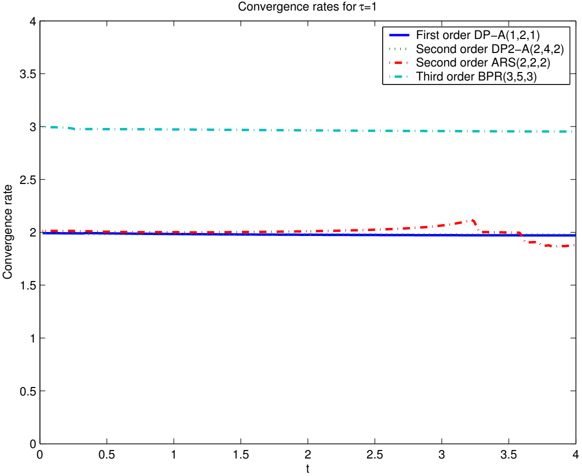
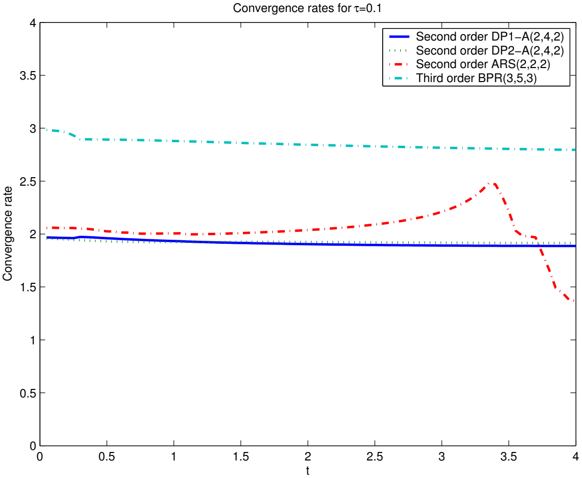
Convergence rates: $\tau = 1$



Convergence rates for various first and second order IMEX schemes for $\tau = 1$.

Convergence rates: $\tau = 0.1$



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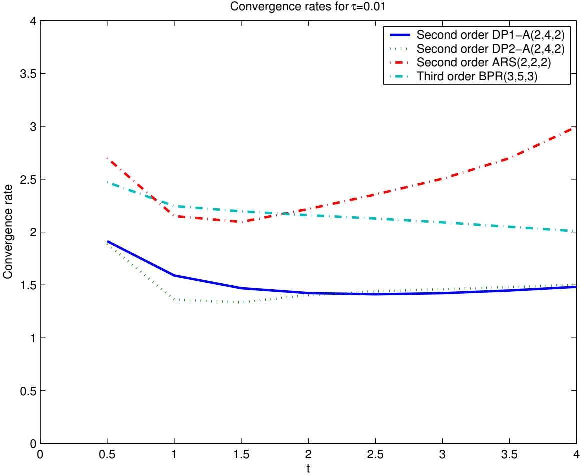

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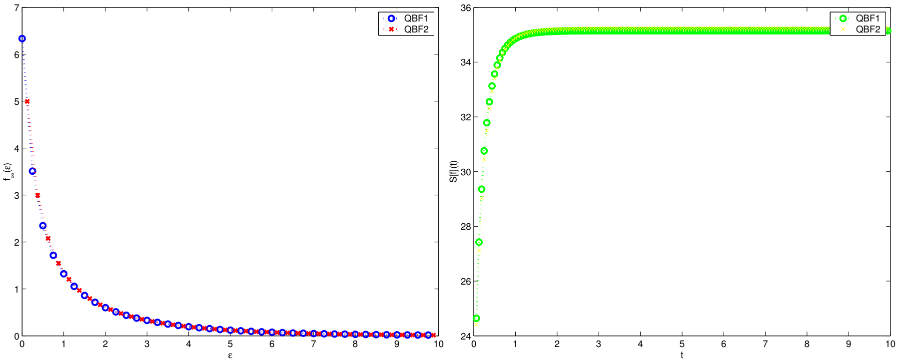
Bose-einstein: Phase-space density

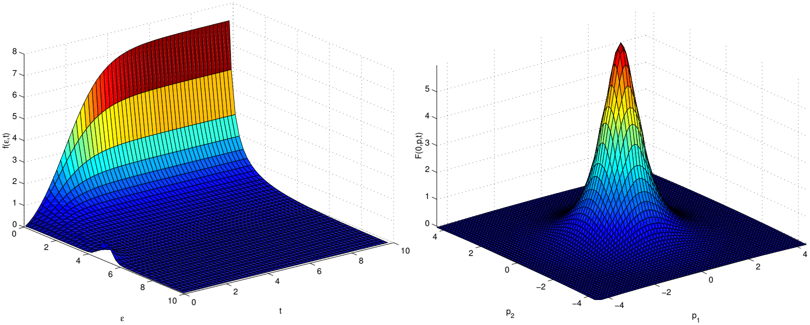
Phase-space density reconstructed at $x = 0$ and $p = (p_1, p_2, 0)$ for scheme QBF2.

Bose-Einstein equilibrium



Stationary discrete Bose-Einstein equilibrium and entropy growth for scheme QBF1 ($\circ$) and QBF2 ($\times$) computed with $N = 40$ points.

Bose-Einstein: Trend to equilibrium



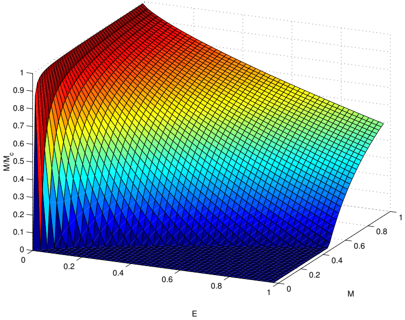
Bose-Einstein: Trend to equilibrium in time for scheme QBF2 (left) with $N = 40$ points and stationary phase-space density reconstructed at $x = 0$ and $p = (p_1, p_2, 0)$ (right).

Condensate mass fraction at equilibrium

We solve numerically for α the equation for E and then compute

$$E = \int_0^\infty \frac{\rho(\varepsilon)\varepsilon}{\exp(\alpha\varepsilon) - 1}\, d\varepsilon \quad \Rightarrow \quad I_\alpha = \int_0^\infty \frac{\rho(\varepsilon)}{\exp(\alpha\varepsilon) - 1}\, d\varepsilon.$$

If $I(\alpha) < M$ the mass entropy pair is critical and condensation will take place. The condensate mass fraction in equilibrium can then be computed $M_c/M = 1 - I_\alpha/M$.



Condensation

In this test we consider the process of condensation of bosons.
We choose the initial distribution in the energy interval $[0, R]$ with $R = 10$ to be[17]

$$f(\epsilon) = \frac{2f_0}{\pi} \arctan(e^{\Gamma(1-\epsilon/\epsilon_0)}),$$

with $\Gamma = 5$ and $\epsilon_0 = R/8$. The dimensionless time scale is

$$\bar{t} = \frac{\varepsilon_0^2 f_0(1+f_0)\sigma m}{\pi^2 \hbar^3} t$$

where $\sigma = 8\pi a^2$ is the total cross section, a the scattering length, m the mass of a particle and $\hbar$ the Planck constant.
We choose $f_0 = 1$ and integrate the Boson Boltzmann equation up to $T = 15$. In this case the mass energy pair is approximatively $(0.42, 0.50)$ which corresponds to a condensate mass fraction of ≈ 0.3 at the stationary state.

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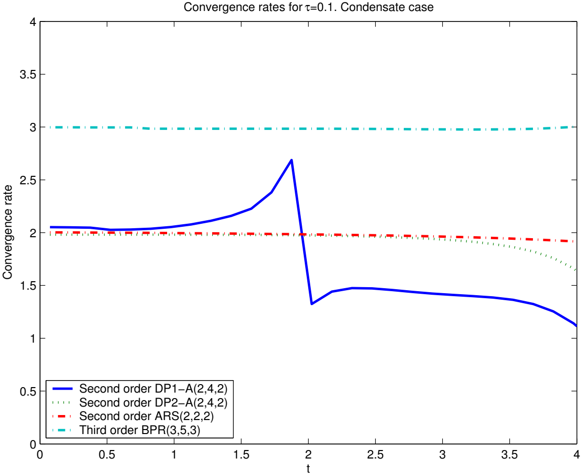

Convergence rates for various first and second order IMEX schemes in the condensate case for $\tau = 0.1$.

Phase-space density (BEC)

Phase-space density reconstructed at $x = 0$ and $p = (p_1, p_2, 0)$ for scheme QBF2.

Summary and future research

- We have developed accurate and AP IMEX schemes for the QBE which avoids the inversion of the implicit collision operator.
- These schemes make the deterministic approach competitive with Monte Carlo methods in terms of computational cost but with an accuracy which is far superior.
- The methods preserve all the relevant physical properties (conservation of mass and energy, entropy inequality and steady states).
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