Thermalization and Bose-Einstein condensation in ultracold atoms

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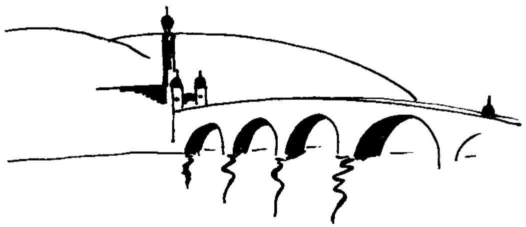

Topics

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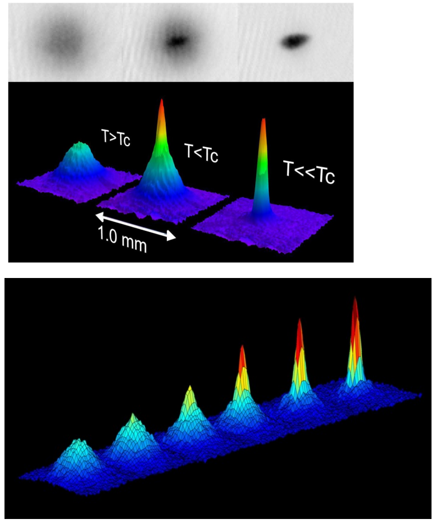
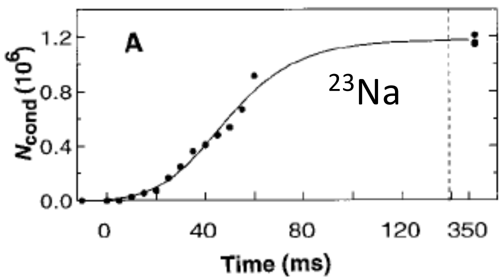
1. Introduction: Cold quantum gases and BEC formation



Time evolution of a ^{87}Rb condensate

1924 Bose, Einstein
1995 BEC: ^{87}Rb (NIST Boulder), ^{23}Na (MIT)
1998 Time dependence of BEC formation (MIT)

- The thermal cloud from which the Bose-Einstein condensate emerges equilibrates subsequent to evaporative cooling
- The time-dependent approach to the equilibrium value of the condensate fraction can be measured, and will be accounted for in a nonequilibrium-statistical model
- The equilibrium condensate fraction depends on the initial temperature T_i , the final temperature T_f , and the initial chemical potential μ_i



H.-J. Miesner et al., Science A 499, 1005 (1998)

The critical temperature is

$$T_c = \frac{2\pi}{m}\left(\frac{n_c}{\zeta(\frac{3}{2})}\right)^{2/3}$$

n_c= critical number density

2. An analytical model for thermalization

The N-body density operator obeys the many-body equation

$$i\,\frac{\partial \hat{\rho}_N(t)}{\partial t} = \left[\hat{H}_{\mathrm{HF}}(t), \hat{\rho}_N(t)\right] + i\hat{K}_N(t)$$

with the Hartree-Fock mean-field part $H_{HF}(t)$, and the collision term $K_N(t)$, which causes the system to thermalize due to two-body collisions. For cold atoms, the trap provides an external potential.

Reducing to the one-body level, the diagonal elements of the ensemble-averaged one-body density operator become

$$\left(\bar{\rho}_1(t)\right)_{\alpha,\alpha} = n(\epsilon_\alpha, t) \equiv n_\alpha(\epsilon, t)$$

with the single-particle occupation numbers n_α^+ for bosons, n_α^- for fermions

The collision term can be written in form of a quantum Boltzmann equation

2.1 Derivation of the nonlinear diffusion equation

Quantum Boltzmann collision term for bosons/ fermions, ergodic approximation

$$\frac{\partial n_1^{\pm}}{\partial t} = \sum_{\epsilon_2,\epsilon_3,\epsilon_4}^{\infty} \langle V_{1234}^2\rangle\, G\left(\epsilon_1+\epsilon_2,\epsilon_3+\epsilon_4\right) \times$$
$$\left[(1\pm n_1)(1\pm n_2)\, n_3\, n_4 - (1\pm n_3)(1\pm n_4)\, n_1\, n_2\right]$$

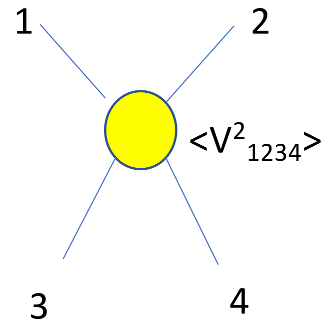
Here: elastic collision kernel

$\langle V_{1234}^2\rangle$ second moment of the interaction

$G\left(\epsilon_1+\epsilon_2,\epsilon_3+\epsilon_4\right)$ energy-conserving function

$\rightarrow \pi\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ in infinite systems

$n_j^{\pm} \equiv n^{\pm}\left(\epsilon_j, t\right)$ occupation number: n^+ bosons, n^- fermions



The Bose-Einstein/ Fermi-Dirac distributions are stationary solutions

$$n_{\text{eq}}^{\pm}(\epsilon) = \frac{1}{e^{(\epsilon-\mu^{\pm})/T} \mp 1}$$

Write the collision term in form of a Master equation (ME) with gain- and loss term

$$\frac{\partial n_1^{\pm}}{\partial t} = (1 \pm n_1) \sum_{\epsilon_4} W^{\pm}_{4\to 1}\, n_4 - n_1 \sum_{\epsilon_4} W^{\pm}_{1\to 4} (1 \pm n_4)$$

with the transition probability ($W_{1\to 4}$ accordingly)

$$W^{\pm}_{4\to 1}(\epsilon_1, \epsilon_4, t) = \sum_{\epsilon_2, \epsilon_3} \langle V^2_{1234} \rangle\, G\,(\epsilon_1 + \epsilon_2, \epsilon_3 + \epsilon_4)\,(1 \pm n_2)\, n_3$$

Introduce the density of states $g_j = g(\varepsilon_j)$; omit ±

$$W_{4\to 1} = W_{41} g_1, W_{1\to 4} = W_{14} g_4$$

$$W_{14} = W_{41} = W\left[\tfrac{1}{2}(\epsilon_4 + \epsilon_1), |\epsilon_4 - \epsilon_1|\right]$$

W is peaked at $\varepsilon_1 = \varepsilon_4$. Obtain an approximation to the ME through a Taylor expansion of n_4 and $g_4 n_4$ around $\varepsilon_1 = \varepsilon_4$ to second order.

Introduce transport coefficients via moments of the transition probability ($x=\varepsilon_4-\varepsilon_1$)

$$D^{\pm}(\epsilon_1,t)=\frac{1}{2}\,g_1\int_0^{\infty}W^{\pm}(\epsilon_1,x)\,x^2dx;\quad v^{\pm}(\epsilon_1,t)=g_1^{-1}\frac{d}{d\epsilon_1}(g_1D^{\pm})$$

and arrive at the nonlinear partial differential equation for the distribution of the occupation numbers $n^{\pm}\equiv n^{\pm}(\epsilon,t)\equiv n^{\pm}(\epsilon_1,t)\equiv n$

$$\frac{\partial n^{\pm}}{\partial t}=-\frac{\partial}{\partial\epsilon}\left[v\,n\,(1\pm n)+n\frac{\partial D}{\partial\epsilon}\right]+\frac{\partial^2}{\partial\epsilon^2}\left[D\,n\right].$$

Nonlinear diffusion equation

Dissipative effects are expressed through the drift term $v(\epsilon,t)$, diffusive effects through the diffusion term $D(\epsilon,t)$.

In the limit of constant transport coefficients, the nonlinear diffusion equation for the occupation-number distribution of bosons/ fermions becomes

$$\frac{\partial n^{\pm}}{\partial t}=-v\,\frac{\partial}{\partial\epsilon}\left[n\,(1\pm n)\right]+D\,\frac{\partial^2 n}{\partial\epsilon^2}$$

G Wolschin, Physica A 499, 1 (2018); A 597, 127299 (2022); EPL 140, 40002 (2022)

The Bose-Einstein/Fermi-Dirac distributions $n^{\pm}_{eq}(\varepsilon)$ are stationary solutions of this equation for constant D, v with the equilibrium temperature (fluctuation-dissipation relation)

$$T = -D/v \text{ with } v < 0$$

Thermalization of cold atoms: Through elastic collisions, the nonlinear evolution pushes a certain fraction of particles from the thermal cloud into the Bose-Einstein condensate. The equilibration time depends on both transport coefficients, $\tau_{eq}(D,v) \propto D/v^2$

The nonlinear boson diffusion equation (NBDE) properly accounts for the thermalization of bosonic atoms provided the boundary condition $n(\varepsilon = \mu < 0) \to \infty$ at the the singularity is introduced.

2.2 Exact solution of the nonlinear diffusion equation

For constant transport coefficients, the solution of the nonlinear diffusion equation for bosons/fermions can be written as the logarithmic derivative

$$n(\epsilon,t) = \pm T\partial_\epsilon \ln \mathcal{Z}(\epsilon,t) \mp \frac{1}{2} = \pm\frac{T}{\mathcal{Z}}\partial_\epsilon \mathcal{Z} \mp \frac{1}{2}$$

of the time-dependent partition function $\mathcal{Z}(\epsilon,t)$

$$\mathcal{Z}(\epsilon,t) = \int_{-\infty}^{+\infty} G(\epsilon,x,t)\, F(x)\, \mathrm{d}x\,,$$

which is an integral over Green's function G (ε, x, t) of the linear diffusion equation

$$\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial \epsilon^2}\right] G(\epsilon,x,t) = \delta(\epsilon - x)\,\delta(t)$$

and an exponential function that contains the initial conditions; for bosons

$$F(x) = \exp\left[-\frac{1}{2D}\left(vx + 2v\,A_{\mathrm{i}}(x)\right)\right].$$

Here, $A_i(x) = \int n_i(y)\,dy$ is the indefinite integral over the initial distribution n_i.
(The integration constant drops out when taking the logarithmic derivative of the partition function.)

For a solution without boundary conditions, Green's function $G_{free}(\varepsilon, x; t)$ is a single Gaussian

$$G_{\rm free}(\epsilon, x, t) = \frac{1}{\sqrt{4\pi D t}} \exp\left[-\frac{(\epsilon - x)^2}{4Dt}\right]$$

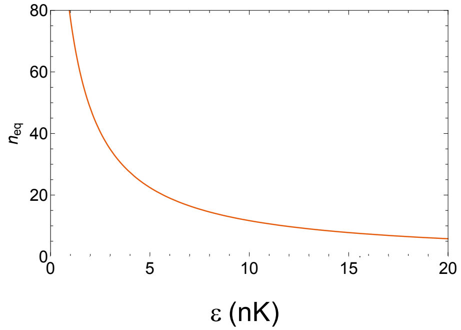
Now, include boundary conditions for bosons at the singularity e = μ, with $\mu_i < 0$ for elastic collisions as determined from particle-number conservation (μ = 0 for inelastic collisions). This requires a new Green's function that equals zero at ε = μ

$$G_{\rm b}(\epsilon, x, t) = G_{\rm free}(\epsilon - \mu, x, t) - G_{\rm free}(\epsilon - \mu, -x, t)\,,$$

and the time-dependent partition function becomes

$$\mathcal{Z}_{\rm b}(\epsilon, t) = \int_0^{+\infty} G_{\rm b}(\epsilon, x, t)\, F(x+\mu)\, {\rm d}x$$

Then we have $\mathcal{Z}_b(\mu, t) = 0$ and $\lim_{\varepsilon\downarrow\mu} n(\varepsilon, t)=\infty\ \forall\ t$ as needed. Moreover, the energy range is restricted to ε ≥ μ.

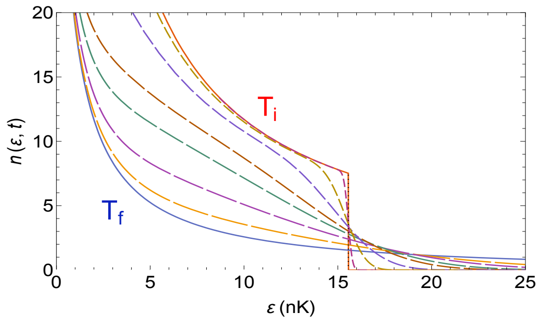


T_i = 130 nK,
μ_i = - 0.67 nK

GW, EPL 129, 40006 (2020)

To conserve particle number during the time evolution for elastic scatterings, a time-varying chemical potential μ(t) is introduced. Once μ(t) reaches zero in the overoccupied case, condensate formation starts. (Particle number is not conserved in the inelastic case with μ = 0.)

Exact solution of the NBDE for a quenched initial distribution



Time-dependent partition function

$$\mathscr{Z} = \sqrt{4Dt}\exp\left(-\frac{\mu}{2T_{\mathrm{f}}}\right)\sum_{k=0}^{\infty}\binom{\frac{T_{\mathrm{i}}}{T_{\mathrm{f}}}}{k}(-1)^k\left(e^{\alpha_k^2 Dt}\left[e^{\alpha_k(\varepsilon-\mu)}\Lambda_1^k(\varepsilon,t) - e^{\alpha_k(\mu-\varepsilon)}\Lambda_2^k(\varepsilon,t)\right] + \exp\left(\frac{(\mu-\varepsilon_i)k}{T_{\mathrm{i}}}\right)\exp\left(\frac{Dt}{4T_{\mathrm{f}}^2}\right)\left[\exp\left(\frac{\varepsilon-\mu}{2T_{\mathrm{f}}}\right)\Lambda_3(\varepsilon,t) - \exp\left(\frac{\mu-\varepsilon}{2T_{\mathrm{f}}}\right)\Lambda_4(\varepsilon,t)\right]\right).$$

$$\alpha_k \equiv \frac{1}{2T_{\mathrm{f}}} - \frac{k}{T_{\mathrm{i}}}$$

$$\Lambda_1^k(\varepsilon,t) \equiv \mathrm{erf}\left(\frac{\varepsilon-\mu+2Dt\alpha_k}{\sqrt{4Dt}}\right) - \mathrm{erf}\left(\frac{\varepsilon-\varepsilon_i+2Dt\alpha_k}{\sqrt{4Dt}}\right)$$

$$\Lambda_2^k(\varepsilon,t) \equiv \mathrm{erf}\left(\frac{\mu-\varepsilon+2Dt\alpha_k}{\sqrt{4Dt}}\right) - \mathrm{erf}\left(\frac{2\mu-\varepsilon-\varepsilon_i+2Dt\alpha_k}{\sqrt{4Dt}}\right)$$

$$\Lambda_3(\varepsilon,t) \equiv \mathrm{erfc}\left(\frac{\varepsilon_i-\varepsilon+tw}{\sqrt{4Dt}}\right)$$

$$\Lambda_4(\varepsilon,t) \equiv \mathrm{erfc}\left(\frac{\varepsilon-2\mu+\varepsilon_i+tw}{\sqrt{4Dt}}\right)$$

Energy-derivative of the partition function

$$\frac{\partial}{\partial\varepsilon}\mathscr{Z} = \sqrt{4Dt}\exp\left(-\frac{\mu}{2T_{\mathrm{f}}}\right)\sum_{k=0}^{\infty}\binom{\frac{T_{\mathrm{i}}}{T_{\mathrm{f}}}}{k}(-1)^k\left(\alpha_k e^{\alpha_k^2 Dt}\left[e^{\alpha_k(\varepsilon-\mu)}\Lambda_1^k(\varepsilon,t) + e^{\alpha_k(\mu-\varepsilon)}\Lambda_2^k(\varepsilon,t)\right] + \exp\left(\frac{(\mu-\varepsilon_i)k}{T_{\mathrm{i}}} + \frac{Dt}{4T_{\mathrm{f}}^2}\right)\frac{1}{2T_{\mathrm{f}}}\left[\exp\left(\frac{\varepsilon-\mu}{2T_{\mathrm{f}}}\right)\Lambda_3(\varepsilon,t) + \exp\left(\frac{\mu-\varepsilon}{2T_{\mathrm{f}}}\right)\Lambda_4(\varepsilon,t)\right]\right)$$

Single-particle distribution function for bosonic atoms

N. Rasch and GW, Phys. Open 2, 100013 (2020)

$$n(\varepsilon,t) = T_{\mathrm{f}}\,(\partial Z(\varepsilon,t)/\partial\varepsilon)\,/\,Z(\varepsilon,t) - 1/2$$

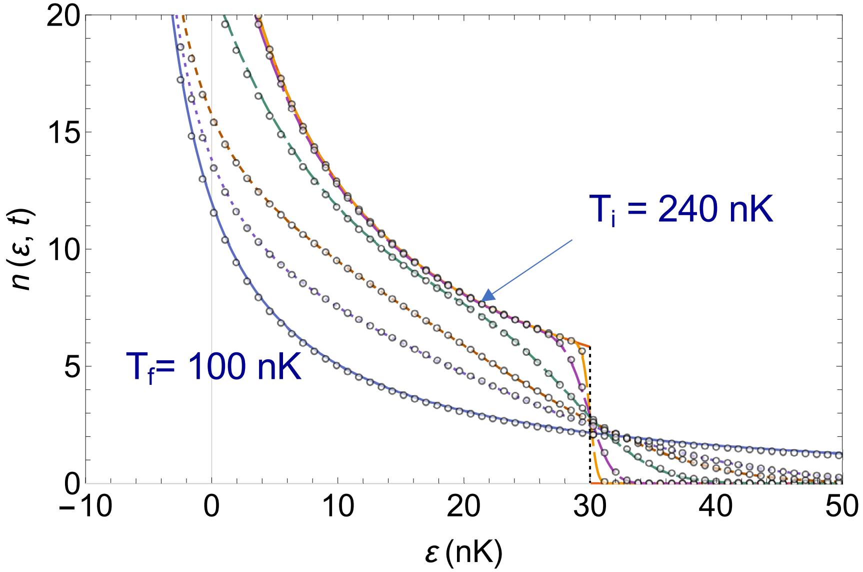
$$\mathcal{Z}(\epsilon,t) = \sqrt{4Dt}\,\exp\left(-\frac{\mu}{2T_{\mathrm{f}}}\right)\sum_{k=0}^{\infty}\binom{\frac{T_{\mathrm{i}}}{T_{\mathrm{f}}}}{k}(-1)^k \times f_k^{T_{\mathrm{i}},T_{\mathrm{f}}}(\epsilon,t)$$

The series terminates for integer T_i/T_f

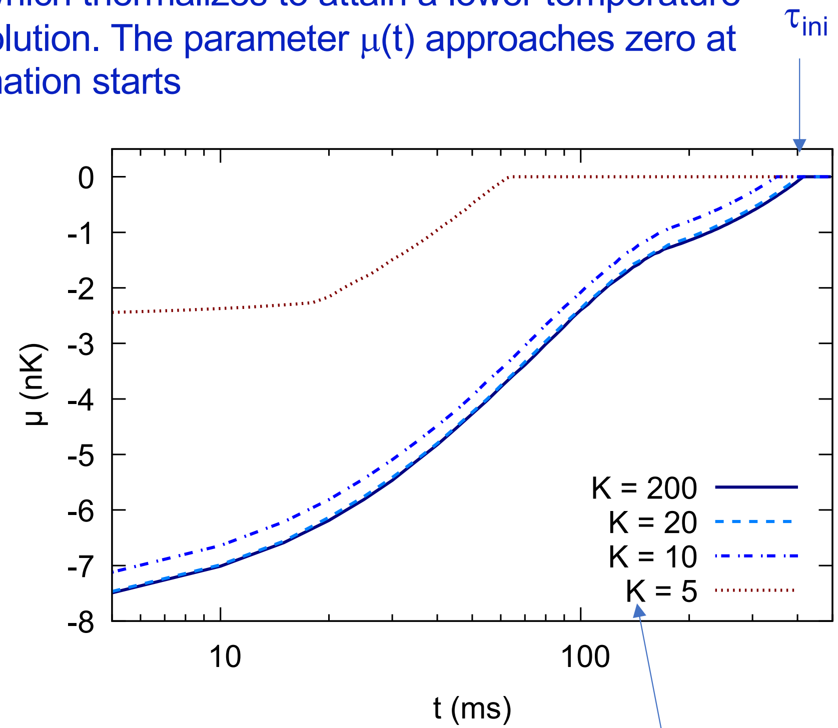
3. Application to ultracold atoms and BEC formation
3.1 Thermalization via elastic scattering

The nonlinear diffusion model is applied to the thermalization of bosonic ultracold atoms, and Bose-Einstein condensate formation subsequent to evaporative cooling

Example: Evaporative cooling of atoms produces a highly nonequilibrium state at an initial temperature of T_i = 240 nK and μ_i = -8 nK, which thermalizes to attain a lower temperature T_f = 100 nK according to the NBDE time evolution. The parameter $\mu(t)$ approaches zero at the initiation time τ_{ini}, when condensate formation starts



--- analytical solutions of the NBDE
o numerical results using Matlab



A. Simon and GW, Physica A 573, 125930 (2021)

3.2 Time-dependent condensate formation in Na-23

The nonlinear diffusion model accounts for the time-dependent Bose-Einstein condensate formation when particle-number conservation is considered in the NBDE

Example: Evaporative cooling of Na-23 atoms, producing a nonequilibrium state at an initial temperature of T_i = 876 nK as in the historical MIT experiment Science 279, 1005 (1998). Time-dependent condensate formation with T_f = 750 nK is compared with our model calculations:

A. Simon and G. Wolschin *Physica A 573 (2021) 125930*

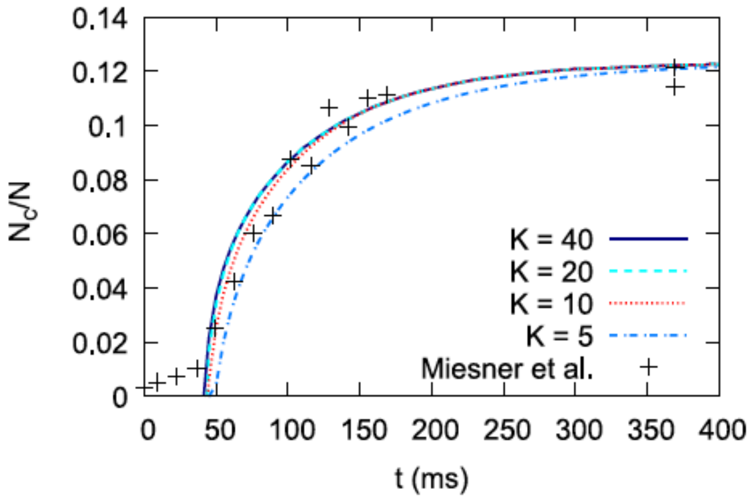


Fig. 7. Condensate fraction $N_c(t)/N$ in an equilibrating Bose gas of ^{23}Na subsequent to fast evaporative cooling in a single step from $T_i = 876$ nK to $T_f = 750$ nK as calculated from the analytical solution of the NBDE Eq. (13) with $k_{max} \equiv K = 5, 10, 20, 40$ in the series expansion of the exact solution, cutoff energy $\epsilon_i = 2190$ nK, $\mu_i = -8$ nK, and the density of states for a free Bose gas. The transport coefficients are $D = 3750$ (nK)^2 ms^{-1}, $v = -5$ nK ms^{-1}. The MIT data for the condensate fraction (crosses, no error bars) are from Ref. [8].

Time-dependent condensate formation in Rb-87

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Growth of Bose-Einstein Condensates from Thermal Vapor

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We report on a quantitative study of the growth process of ^{87}Rb Bose-Einstein condensates. By continuous evaporative cooling we directly control the thermal cloud from which the condensate grows. We compare the experimental data with the results of a theoretical model based on quantum kinetic theory. We find quantitative agreement with theory for the situation of strong cooling, whereas in the weak cooling regime a distinctly different behavior is found in the experiment.

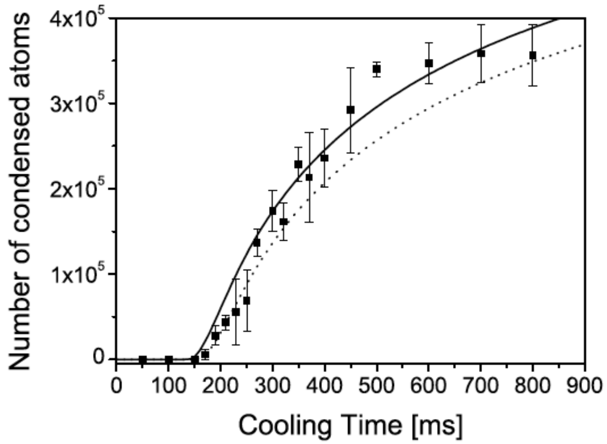


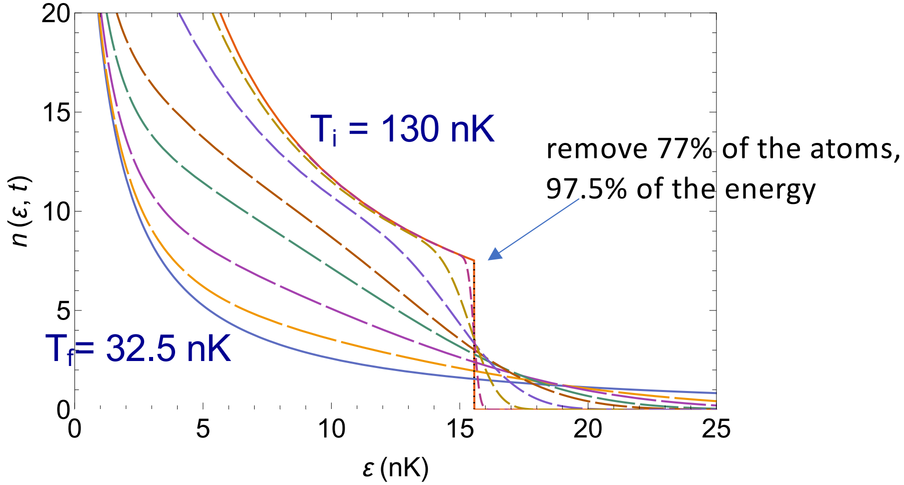
FIG. 1. Growth curve of a Bose-Einstein condensate for an evaporation parameter $\eta = 1.4$. The lines are the results of the numerical simulation of the growth for the starting conditions $N_i = 4.4 \times 10^6$ and $T_i = 610$ nK (solid) and $N_i = 4.2 \times 10^6$ and $T_i = 610$ nK (dotted). Every data point is averaged over three identical repetitions of the experiment with statistical errors shown by the bars.

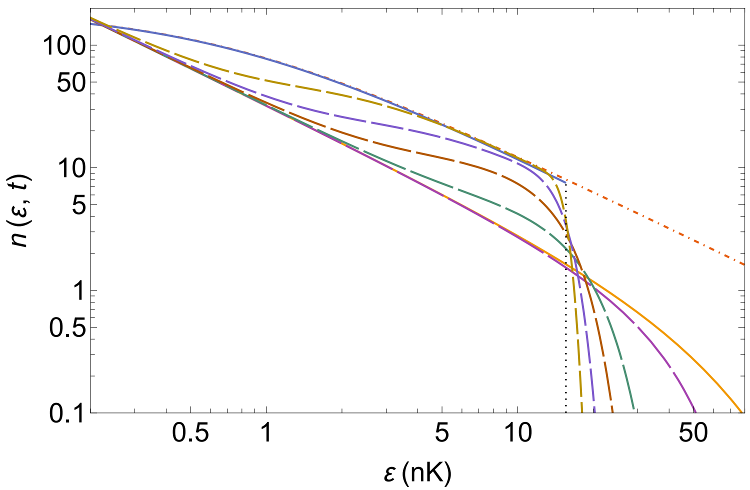
Continuous evaporative cooling resulting in BEC formation: Excellent time resolution.

3.3 Thermalization and condensate formation in K-39: Deep quench

The nonlinear diffusion model is best suited to account for the thermalization of bosonic ultracold atoms, and Bose-Einstein condensate formation in case of a deep quench (instead of gradual evaporative cooling)

Example: Deep quench in K-39 atoms, producing a highly nonequilibrium state at an initial temperature of T_i = 130 nK as in the Cambridge experiment Nature Phys. 17, 457 (2021). Time-dependent condensate formation is measured for various scattering lengths, and compared to our model calculations:



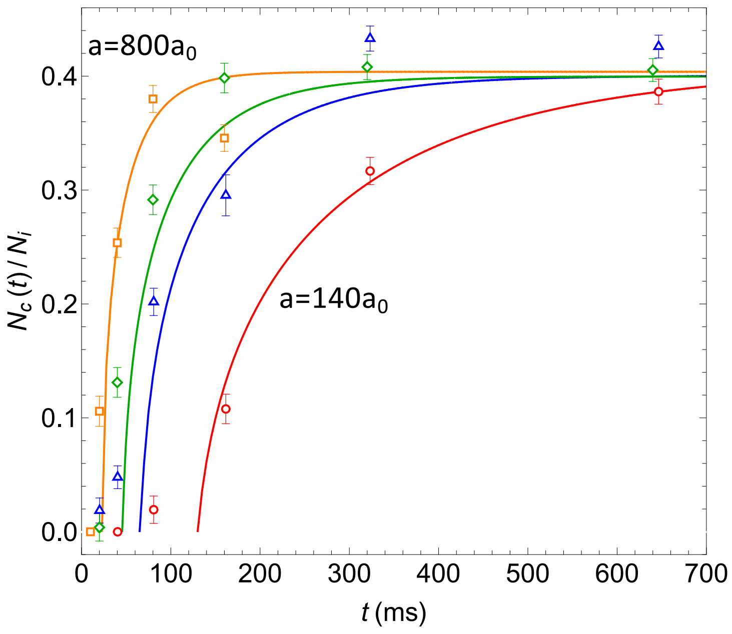


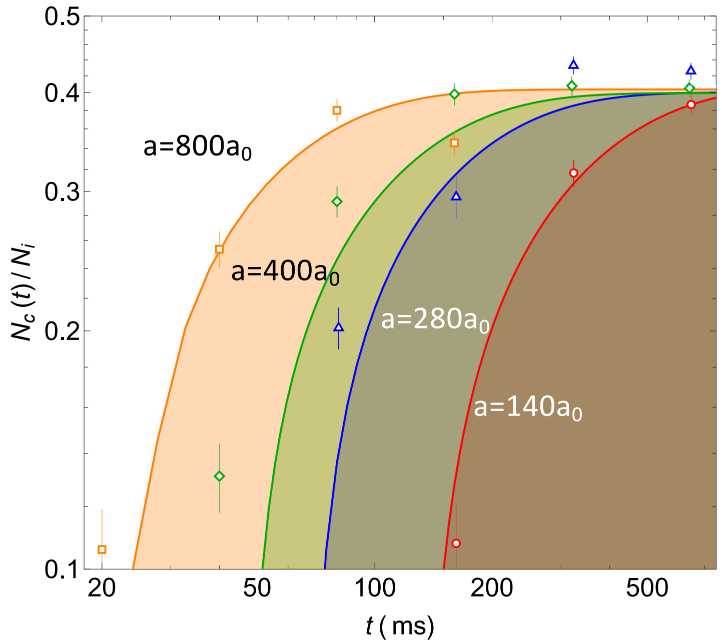
A. Kabelac and GW, Eur.Phys.J. D76, 178 (2022)

Time-dependent condensate formation in K-39 vapour at various interaction energies

The nonlinear diffusion model can be applied to the time-dependent Bose-Einstein condensate formation.
Here, particle number is conserved following the deep quench:

$N_i = N_{th}(t) + N_c(t) = \int n(\varepsilon,t)\, g(\varepsilon)\, d\varepsilon + N_c(t) \Rightarrow$ Condensate fraction $\equiv N_c(t)/N_i = 1 - N_{th}(t)/N_i$





a_0 = Bohr radius ≈ 0.0529 nm
a = s-wave scattering length

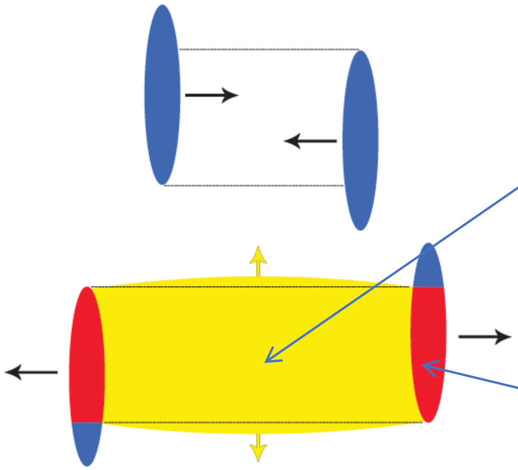
[39]K Data from J.A.P. Glidden et al., Nature Phys. 17, 457-461 (2021). **GW, EPL 140, 40002 (2022)**

Table 1 Transport coefficients, initiation and equilibration times for BEC formation in ^{39}K

($T_\mathrm{i} = 130$ nK, $T_\mathrm{f} = -D/v = 32.5$ nK)

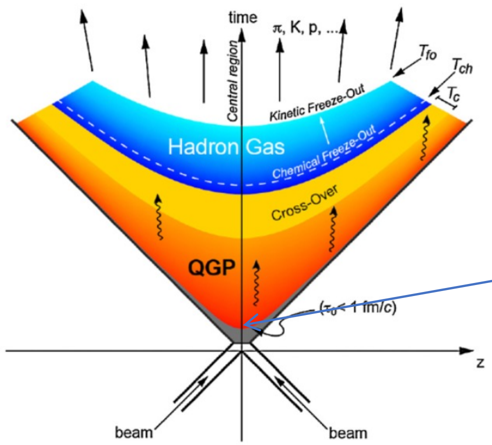
$a\,(a_\infty)$	$D\,(\mathrm{nK}^2/\mathrm{ms})$	$v\,(\mathrm{nK}/\mathrm{ms})$	τ_ini (ms)	τ_eq (ms)
140	0.08	−0.00246	130	600
280	0.16	−0.00492	65	300
400	0.229	−0.00705	46	210
800	0.457	−0.01406	23	105

4. Epilog: Thermalization in the initial stages of relativistic heavy-ion collisions



Fast local equilibration of gluons in the fireball (QGP) towards the Bose-Einstein distribution (Global thermodynamic equilibrium is usually not attained). This is as prerequisite for subsequent hydrodynamic expansion, cooling and hadronization.

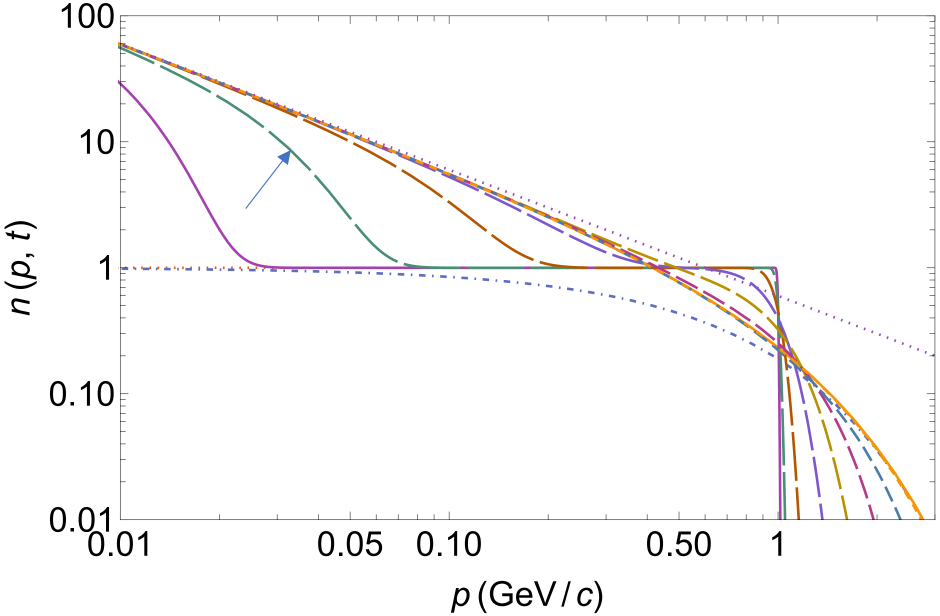
Local equilibration of quarks in the fragmentation sources towards the Fermi-Dirac distribution



Spacetime diagram for the evolution of the QGP

Pre-equilibrium phase, τ_{eq}< 1 fm/c;
typical interaction time ≈ 5-8 fm/c

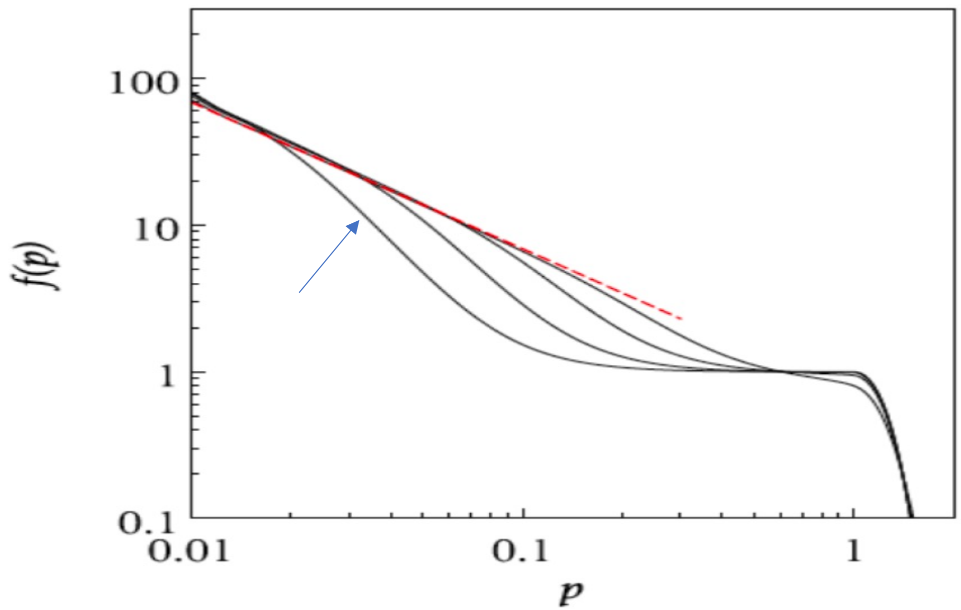
Comparison with a numerical thermalization model for μ=0, n_i^0=1
(NBDE solutions for inelastic collisions vs. Blaizot et al.)



NBDE solutions: Time-dependent single- particle occupation-number distribution functions n(p,t) at $t = 2 \times 10^{-5}$, 2×10^{-4} , 2×10^{-3} , 0.01, 0.04, 0.12, 0.4 and 2 fm/c (decreasing dash lengths).

n_i^0=1.0; T = 600 MeV (solid curve, BE-distribution)
D = 1.2 GeV^2 /fm, v = −2 GeV/fm

G. Wolschin, Physica A 597, 127299 (2022)



Numerical QCD-based calculations of the **soft (IR) modes only** at early times $t \approx 2 \times 10^{-4}$, 8×10^{-4} , 3×10^{-3}, 0.01 fm/c (with n_i^0=1.0, T=690 MeV) from:
J.-P. Blaizot, J. Liao, Y. Mehtar-Tani, NPA 961, 37 (2017):

This numerical model in the small-angle approximation agrees reasonably well with the analytical NBDE-approach in the IR

5. Summary and Conclusion

- From the quantum Boltzmann collision term, a nonlinear partial differential equation for the time-dependent occupation-number distribution in a finite Fermi/ Bose system is derived

- The nonlinear boson diffusion equation (NBDE) is solved analytically including the boundary conditions at the singularity

- The solution accounts for the thermalization of ultracold atoms and time-dependent Bose-Einstein condensate formation such as in K-39

- The model can also be applied to the thermalization of quarks and gluons in the initial stages of relativistic heavy-ion collisions, and other nonequilibrium processes in physics.

Thank you for your attention !