Thermalization and Bose-Einstein condensation of ultracold atoms

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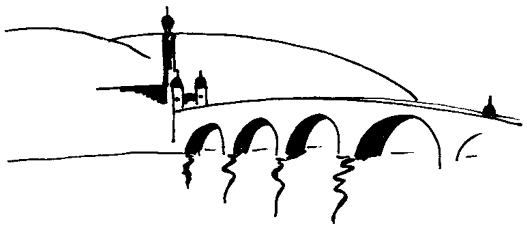

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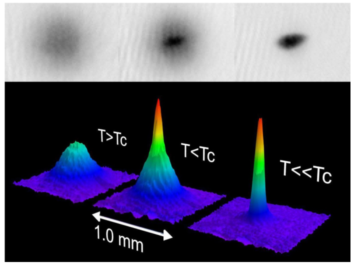
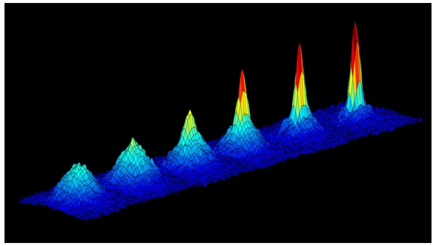
1. Introduction: Cold quantum gases and BEC formation

- 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



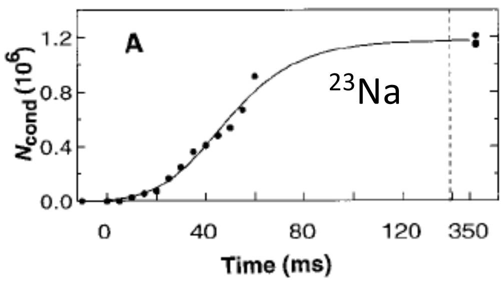


Time evolution of a ^{87}Rb condensate

1924 Bose, Einstein

1995 BEC: ^{87}Rb (NIST Boulder), ^{23}Na (MIT)

1998 Time dependence of BEC formation (MIT)



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

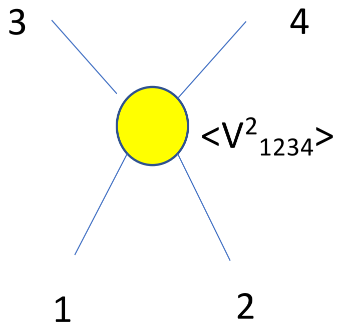
$$i\frac{\partial\hat{\rho}_N(t)}{\partial t} = [\hat{H}_{\mathrm{HF}}(t),\hat{\rho}_N(t)] + i\hat{K}_N(t) \qquad \big(\bar{\rho}_1(t)\big)_{\alpha,\alpha} = n(\epsilon_\alpha,t) \equiv n_\alpha(\epsilon,t)$$

2.1 Derivation of the nonlinear diffusion equation

Quantum Boltzmann collision term for bosons/ fermions, ergodic approximation

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

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

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

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

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

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

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

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

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 $n^{\pm}\equiv n^{\pm}(\epsilon,t)\equiv n^{\pm}(\epsilon_1,t)\equiv n$

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

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

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

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

The Bose-Einstein/Fermi-Dirac distributions $n^{\pm}_{eq}(\varepsilon)$ are stationary solutions of this equation with the equilibrium temperature

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

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 at any given value of the energy depends on both transport coefficients, $\tau_{eq}(D,v)$.

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

2.2 Exact solution of the nonlinear equation

The solution of the NBDE for single-particle bosonic level occupation probabilities n(ε,t) can be written as the logarithmic derivative

$$n(\epsilon, t) = T \frac{\partial}{\partial \epsilon} \ln \mathcal{Z}(\epsilon, t) - \frac{1}{2} = T \frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \epsilon} - \frac{1}{2}$$

of the time-dependent partition function

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

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

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

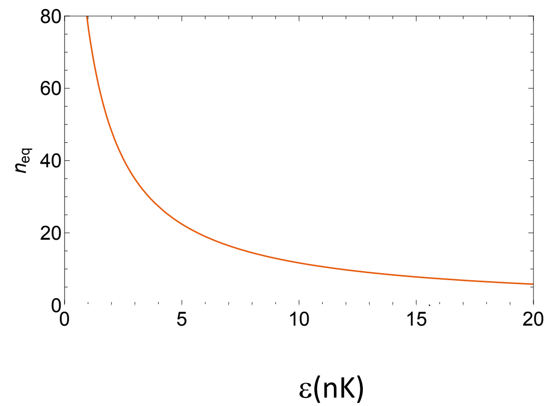
Here, $A_i(x) = \int n_i(y)\, dy$ is the indefinite integral over the initial distribution n_i.
(The integration constant drops out when taking the logarithmic derivative of the partition function.)

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

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

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

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



T_i = 130 nK,
μ_i = - 0.67 nK

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

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

G Wolschin, EPL 129, 40006 (2020)

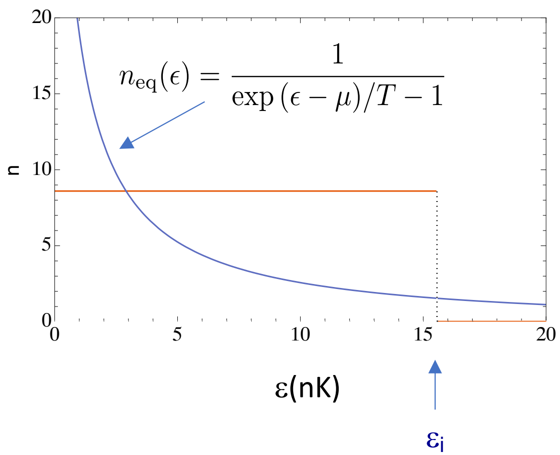
Equilibration time for bosons vs. fermions

An explicit expression for the bosonic equilibration time at the cut ε_i follows from an asymptotic expansion of the error functions occuring in the analytical solutions for theta-function initial distributions with boundary ε_i

$$\mathrm{erf}\,(z_\mathrm{b}) \simeq 1 - \frac{1}{\sqrt{\pi}\, z_\mathrm{b}} \exp\left[-z_\mathrm{b}^2\right] + \exp(-z_\mathrm{b}^2)\, \mathcal{O}\left(\frac{1}{z_\mathrm{b}^3}\right)$$

with argument z_b at the boundary ε_i for an initial box distribution

$$z_b = \frac{1}{2\sqrt{D}}[\epsilon_\mathrm{i} - \epsilon + 3vt]$$



Deviations from the thermal solution thus scale with

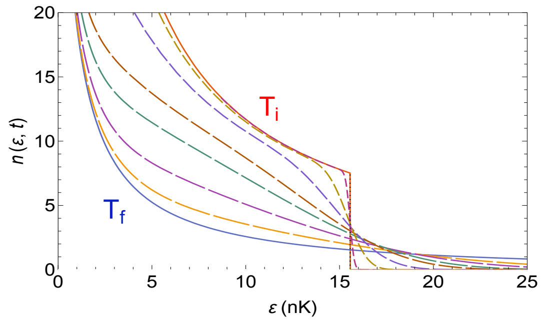
$$\exp[-9v^2 t/(4D)] \equiv \exp[-t/\tau_\mathrm{eq}]$$

and the equilibration time in a Bose system at the cut becomes

$$\boxed{\tau_\mathrm{eq}^\mathrm{Bose} = 4D/(9v^2) = \tau_\mathrm{eq}^\mathrm{Fermi}/9}$$

GW, Physica A 499, 1 (2018)

For an arbitrary initial distribution $n_i(\varepsilon)$, the equilibration time becomes $\tau_{eq} \propto f\, D/v^2$



Exact solution of the NBDE for a quenched initial distribution

Time-dependent partition function

$$\mathcal{Z} = \sqrt{4Dt}\,\exp\left(-\frac{\mu}{2T_f}\right)\sum_{k=0}^{\infty}\begin{pmatrix}\frac{T_i}{T_f}\\ k\end{pmatrix}(-1)^k\left(e^{\alpha_k^2 Dt}\left[e^{\alpha_k(\varepsilon-\mu)}\Lambda_1^k(\varepsilon,t) - e^{\alpha_k(\mu-\varepsilon)}\Lambda_2^k(\varepsilon,t)\right] + \exp\left(\frac{(\mu-\varepsilon_i)k}{T_i}\right)\exp\left(\frac{Dt}{4T_f^2}\right)\left[\exp\left(\frac{\varepsilon-\mu}{2T_f}\right)\Lambda_3(\varepsilon,t) - \exp\left(\frac{\mu-\varepsilon}{2T_f}\right)\Lambda_4(\varepsilon,t)\right]\right).$$

$$\alpha_k \equiv \frac{1}{2T_f} - \frac{k}{T_i}$$

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

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

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

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

Energy-derivative of the partition function

$$\frac{\partial}{\partial\varepsilon}\mathcal{Z} = \sqrt{4Dt}\,\exp\left(-\frac{\mu}{2T_f}\right)\sum_{k=0}^{\infty}\begin{pmatrix}\frac{T_i}{T_f}\\ k\end{pmatrix}(-1)^k\left(\alpha_k e^{\alpha_k^2 Dt}\left[e^{\alpha_k(\varepsilon-\mu)}\Lambda_1^k(\varepsilon,t) + e^{\alpha_k(\mu-\varepsilon)}\Lambda_2^k(\varepsilon,t)\right] + \exp\left(\frac{(\mu-\varepsilon_i)k}{T_i} + \frac{Dt}{4T_f^2}\right)\frac{1}{2T_f}\left[\exp\left(\frac{\varepsilon-\mu}{2T_f}\right)\Lambda_3(\varepsilon,t) + \exp\left(\frac{\mu-\varepsilon}{2T_f}\right)\Lambda_4(\varepsilon,t)\right]\right)$$

Single-particle distribution function for bosonic atoms

$$\boxed{n(\varepsilon,t) = T_f\,(\partial Z(\varepsilon,t)/\partial\varepsilon)\,/\,Z(\varepsilon,t) - 1/2}$$

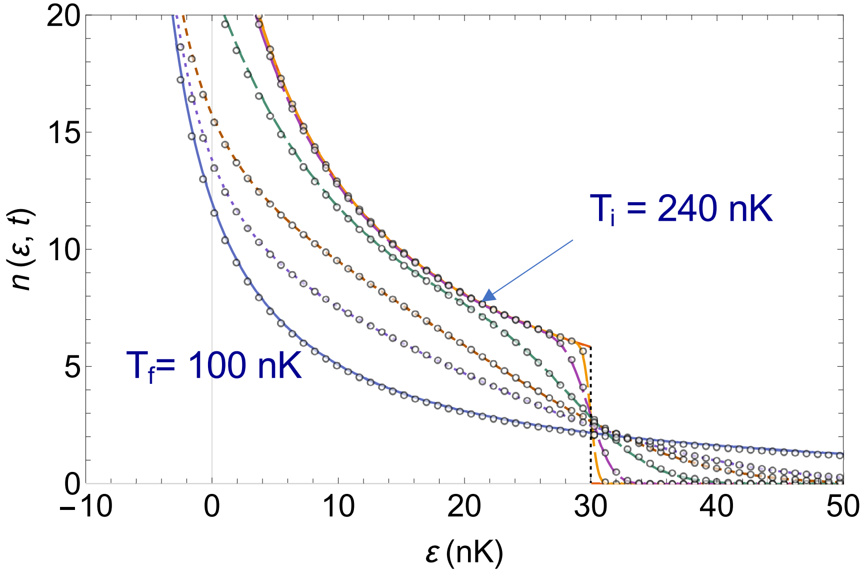
N. Rasch and GW, Phys. Open 2, 100013 (2020)

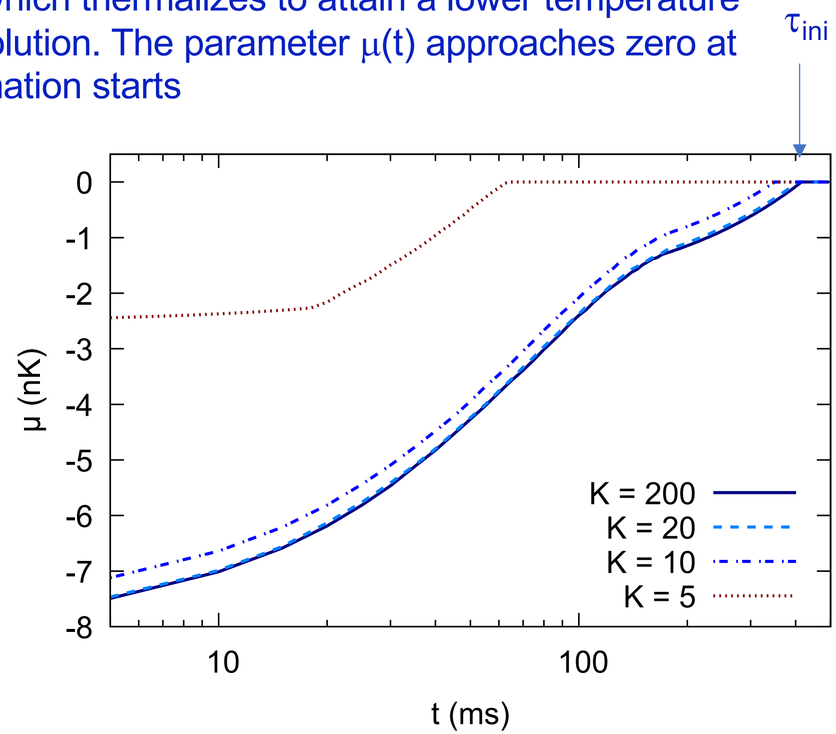
3. Application to ultracold atoms and BEC formation

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 is particularly suited to account 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 that include particle-number conservation:

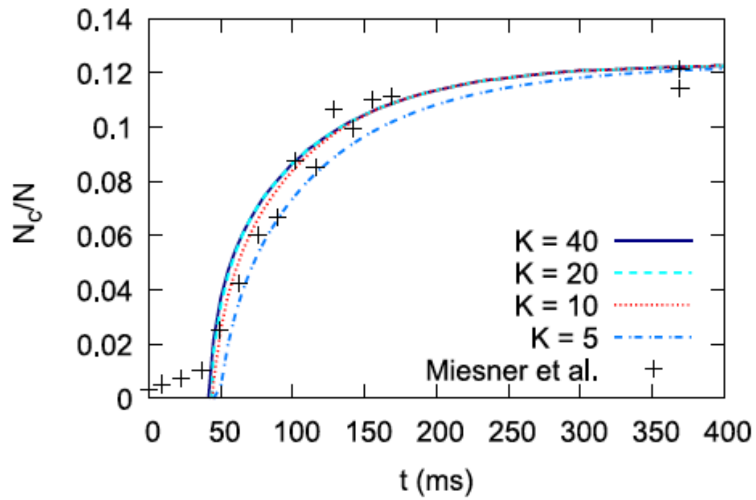


Fig. 7. Condensate fraction $N_c(t)/N$ in an equilibrating Bose gas of ^{23}Na subsequent to fast evaporative cooling in a single step from $T_i = 876$ nK to $T_f = 750$ nK as calculated from the analytical solution of the NBDE Eq. (13) with $k_{max} \equiv K = 5, 10, 20, 40$ in the series expansion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

$N_c(t) = N_i - N_{th}(t)$

$N_c(t)/N_i = 1 - N_{th}(t)/N_i$

"Condensate fraction"

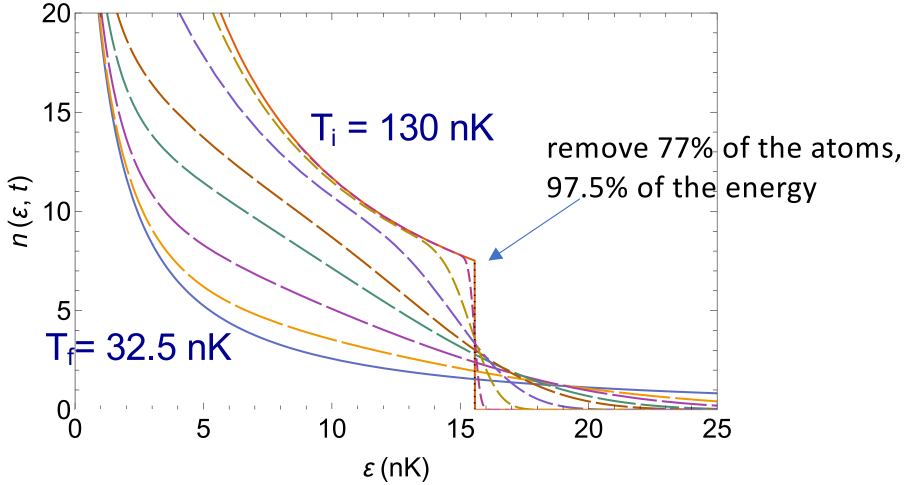
$N_{th}(t) = \int n(\varepsilon,t)\, g(\varepsilon)\, d\varepsilon$

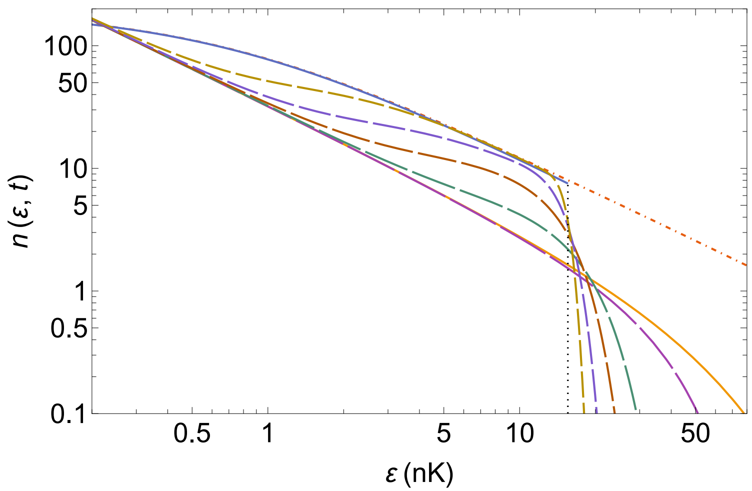
Physica A 573, 125930 (2021)

3.3 Thermalization and condensate formation in K-39

The nonlinear diffusion model is particularly 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:





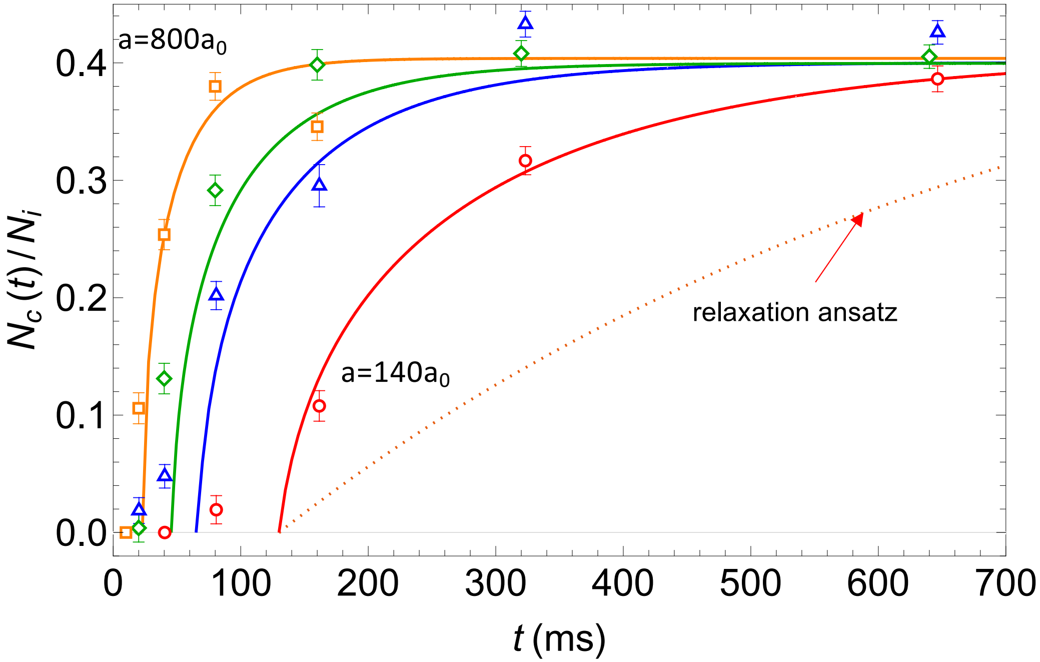
T_i / T_f = 4: infinite series terminates!

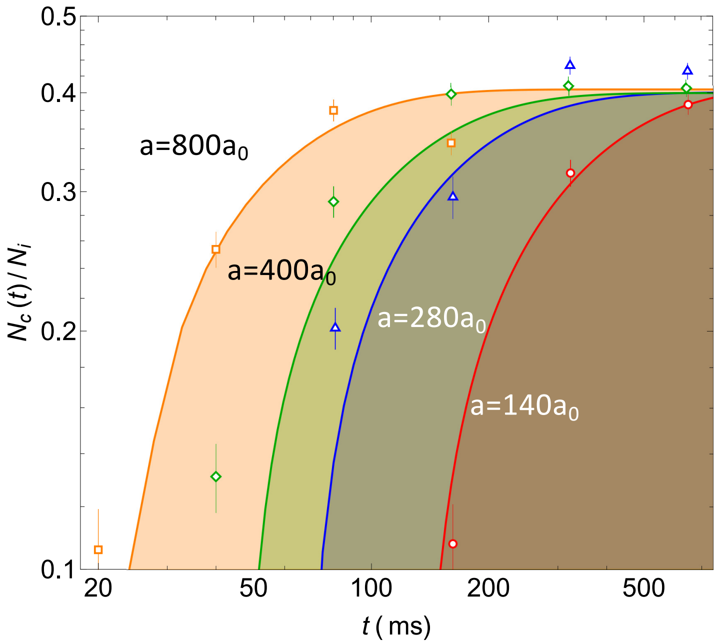
A. Kabelac and GW, Eur. Phys. J. D76, 178 (2022)

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). G Wolschin, submitted to EPL (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

$$\boxed{D, v \propto a\ ;\ \tau_{\mathrm{ini}}, \tau_{\mathrm{eq}} \propto 1/a}$$

$$D = \quad f\,T_{\mathrm{f}}^2/\tau_{\mathrm{eq}} \simeq 0.08\,(\mathrm{nK})^2/\mathrm{ms}\,,$$

$$v = -f\,T_{\mathrm{f}}/\tau_{\mathrm{eq}} \simeq -0.00246\,\mathrm{nK}/\mathrm{ms}$$

f = 0.045

4. 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

- 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 !