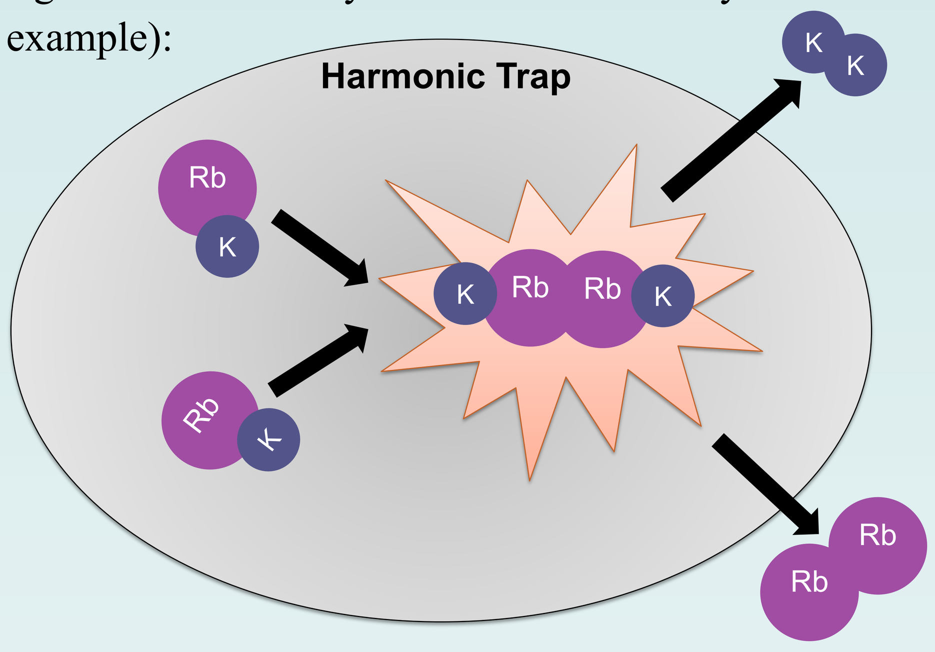
Ultracold Chemical Reaction in Single-Component Fermi Gases

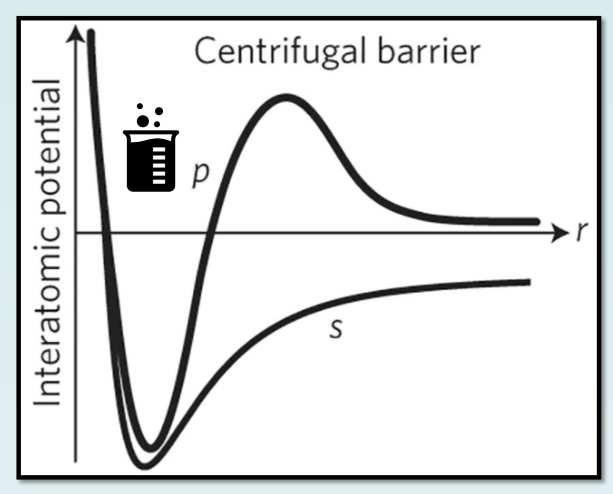
Xin-Yuan Gao[1], D. Blume[2,3], and Yangqian Yan[1,4]

[1] Department of Physics, The Chinese University of Hong Kong
[2] Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma
[3] Center for Quantum Research and Technology, The University of Oklahoma
[4] The Chinese University of Hong Kong Shenzhen Research Institute

Introduction

In recent years, the creation of ultracold molecular gases has revolutionized the field of quantum simulation. Concurrently, the intrinsic non-Hermitian decay dynamics observed within these systems have carved out a novel niche in quantum chemistry. Fermionic single-component molecular gas is one of the simplest systems as an example. The experimental realizations include $^{40}K^{87}Rb$ molecular gas [1] and $^{23}Na^{40}K$ molecular gas [2]. Besides fermionic statistics and weak elastic interaction, which seems boring, the ***p*-wave** two-body loss, a typical feature in such systems, makes them non-trivial and suitable for studying non-Hermitian dynamics. The two-body loss comes from the **chemical reaction** (We use $^{40}K^{87}Rb$ as an example):





The large energy released from the reaction will be converted to the kinetic energy of outgoing products, allowing them to leave the trap almost immediately. Thus, by monitoring the total number of particles that remain in the system $N(t)$, the loss dynamics can be studied. What kind of equation of motion does $N(t)$ obey? Most naively, one always guess

$$\partial_t N(t) = -\beta N(t)^2$$

since the chemical reaction is a **two-body process**. This phenomelogical conjecture has been widely used in analyzing various experimental results. Sometimes it works, while it also yields confusing results in some cases. Our work tends to answer the following question about above two-body model:

1) Is β a constant? How can we calculate β?
2) Is the model a good one for capturing the main feature of ultracold chemical reaction in single-component Fermi gases. Does the model always work?
3) What is the influence from the harmonic trap to the system, which is usually adopted in realistic experiments?

Methodology

p-wave Contact and Two-Body Loss Rate [3]

(Generalized) Tan's contact is the thermodynamics quantity conjugated to p-wave scattering volume.

$$C_v = -\frac{2m}{3\hbar^2}\frac{\partial\Omega}{\partial v_p^{-1}}$$

The contact can be directly related to the two-body loss rate by

$$\frac{\mathrm{d}N}{\mathrm{d}t} = \frac{6\hbar}{m}C_v\frac{\mathrm{Im}(v_p)}{[\mathrm{Re}(v_p)]^2}$$

Equation of States of p-wave Fermi Gas [4]

We find the analytical form of the equation of state of p-wave Fermi gas:

$$\frac{\Omega}{k_BTV} = \frac{\mathrm{Li}_{5/2}(-z)}{\lambda_T^3} + \frac{18\pi v_p \mathrm{Li}_{3/2}(-z)\mathrm{Li}_{5/2}(-z)}{\lambda_T^6}$$

$$n = -\frac{\mathrm{Li}_{3/2}(-z)}{\lambda_T^3} - \frac{18\pi v_p[\mathrm{Li}_{3/2}(-z)^2 + \mathrm{Li}_{1/2}(-z)\mathrm{Li}_{5/2}(-z)]}{\lambda_T^6}$$

Inelastic Quantum Boltzmann Equation [4]

We derive that the quantum dynamics of such systems can be fully described by a quantum version of the transport Boltzmann equation

$$\frac{dn_{\mathbf{k}}}{dt} = \mathcal{I}_{\rm inel}[n_{\mathbf{k}}] + \mathcal{I}_{\rm el}[n_{\mathbf{k}}]$$

where the inelastic and elastic collision integrals are

$$\mathcal{I}_{\rm inel}[n_{\mathbf{k}}] = \frac{12\pi\hbar\mathrm{Im}(v_p)V}{m}\int\frac{d^3q}{(2\pi)^3}(q^2+k^2)n_{\mathbf{k}}n_{\mathbf{q}},$$

$$\mathcal{I}_{\rm el}[n_{\mathbf{k}}] = \frac{288\pi^3\hbar\mathrm{Re}(v_p)^2V^3}{m}\int\frac{d^3q}{(2\pi)^3}\int\frac{d^3Q}{(2\pi)^3}\delta(k^2-q^2+\mathbf{k}\cdot\mathbf{Q}-\mathbf{q}\cdot\mathbf{Q})$$
$$\times\left(\frac{\mathbf{Q}}{2}-\mathbf{k}\right)^2\left(\frac{\mathbf{Q}}{2}-\mathbf{q}\right)^2[(1-n_{\mathbf{Q}-\mathbf{k}})(1-n_{\mathbf{k}})n_{\mathbf{q}}n_{\mathbf{Q}-\mathbf{q}} - n_{\mathbf{Q}-\mathbf{k}}n_{\mathbf{k}}(1-n_{\mathbf{q}})(1-n_{\mathbf{Q}-\mathbf{q}})].$$

Local Density Approximation

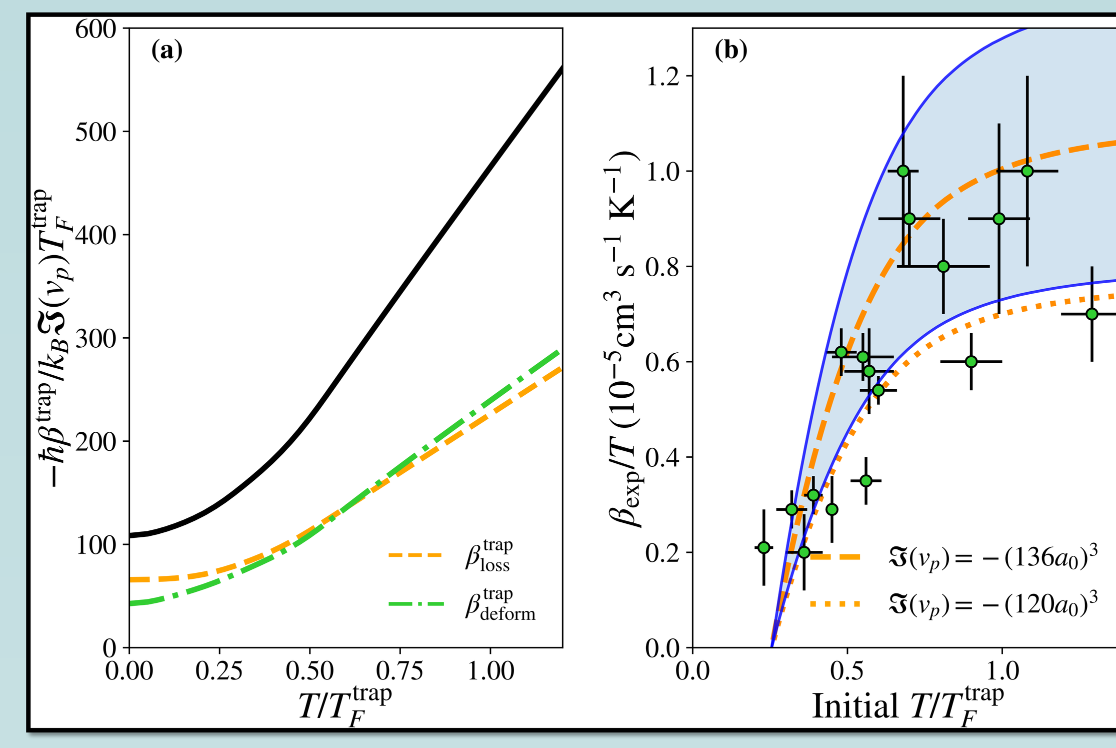
In the thermodynamic limit, we can translate our homogeneous results to those for harmonically trapped systems.

$$n_{\mathbf{k}} \to \int d^3r f(\mathbf{k},\mathbf{r}) \qquad \frac{df}{dt} = \left[-\frac{\hbar\mathbf{k}}{M}\nabla_{\mathbf{r}} + \frac{\nabla_{\mathbf{r}}U_{\rm ext}\cdot\nabla_{\mathbf{k}}}{\hbar}\right]f + \frac{\mathcal{I}_{\rm inel}[f]}{V} + \frac{\mathcal{I}_{\rm el}[f]}{V^3}$$

Results

Answer to Q(1): Temperature-Dependent β for Equilibrium Systems [3]

Since p-wave contact is temperature-dependent, the two-body loss rate coefficient β also varies against temperature.



Lines are our theoretical predictions, and green scatters are experimental data from Ref. [2]

Answer to Q(2): Two-Body Loss Dynamics for Non-Equilibrium Homogeneous System [4]

Contact is a thermodynamics quantity defined only for equilibrium systems. When the elastic collision is weak enough, the system cannot always be assumed to be in equilibrium. By solving the inelastic Boltzmann equation analytically, we find a precise approximation for any initial temperature:

$$N(t) = N(0)\left[1+\left(F_1(0)+\frac{F_2(0)}{F_1(0)}\right)\tau\right]^{\frac{-2F_1(0)^2}{F_1(0)^2+F_2(0)}}, \quad \tau = -\frac{12\pi\hbar k_F^5\mathrm{Im}(v_p)t}{m}$$

where

$$F_j(0) = -\frac{3}{2}\left(\frac{T}{T_F(0)}\right)^{\frac{3}{2}+j}\Gamma(\frac{3}{2}+j)\mathrm{Li}_{\frac{3}{2}+j}[-z(T)].$$

The result can be interpreted as the solution of the following equation of motion:

$$\frac{dN(t)}{dt} \propto -N(t)^{\mathcal{N}},$$

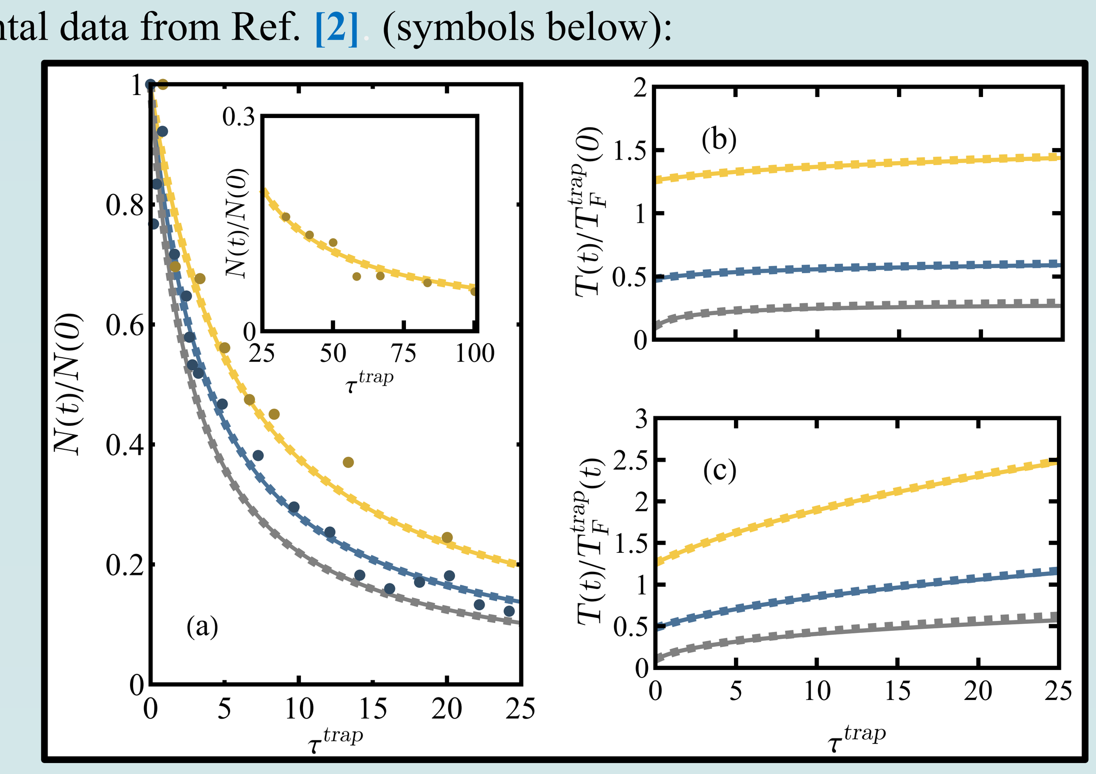
where

$$\mathcal{N} = 3/2 + \frac{F_2(0)}{2F_1(0)^2}$$

Two Limits: $\mathcal{N} \xrightarrow{T\to\infty} \frac{7}{3}, \quad \mathcal{N} \xrightarrow{T\to 0} \frac{44}{21}$

Answer to Q(3): Harmonic Trap Suppression of $\mathcal{N}$ [4]

Generally, we can numerically solve the inelastic Quantum Boltzmann equation by separating two different time scales of inhomogeneous flow and two-body loss. We show that our calculation compares well with experimental data from Ref. [2] (symbols below):



A rather precise approximation for (initial) high-temperature solutions of inelastic Quantum Boltzmann equation is

$$C = 0.198418/\sqrt{T(0)/T_F^{\rm trap}(0)}, \quad \tau^{\rm trap} = -\frac{\hbar[k_F^{\rm trap}(0)]^5}{\pi M}\mathrm{Im}(v_p)t$$

$$N(t) = N(0)/\left[1+C\tau^{\rm trap}\right]^{0.96},$$
$$T(t) = T(0)\left[1+C\tau^{\rm trap}\right]^{0.08},$$
$$\frac{T(t)}{T_F^{\rm trap}(t)} = \frac{T(0)}{T_F^{\rm trap}(0)}\left[1+C\tau^{\rm trap}\right]^{0.4}$$

$$\mathcal{N} = 2.04167$$

Acknowledgements and References

This work is supported by the National Natural Science Foundation of China under Grant No. 12204395, Hong Kong RGC Early Career Scheme under Grant No. 24308323, and the National Science Foundation (NSF) under Grant No. PHY-2110158.

References:

[1] L. De Marco, G. Valtolina, K. Matsuda, W. G. Tobias, J. P. Covey, and J. Ye, A degenerate Fermi gas of polar molecules, Science 363, 853 (2019).
[2] M. Duda, X.-Y. Chen, R. Bause, A. Schindewolf, I. Bloch, and X.-Y. Luo, Long-Lived Fermionic Feshbach Molecules with Tunable p-Wave Interactions, Phys. Rev. A 107, 053322 (2023).
[3] X.-Y. Gao, D. Blume, and Y. Yan, Temperature-Dependent Contact of Weakly Interacting Single-Component Fermi Gases and Loss Rate of Degenerate Polar Molecules, Phys. Rev. Lett. 131, 043401 (2023).
[4] Our manuscripts under preparation