DEGENERATE FERMI GASES AT ENS: THEORY AND EXPERIMENTS

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OUTLINE

- Present experiments with fermions: why interesting ?
- Feshbach resonance: which model for the interaction potential ?
- A very simple model: a matter wave with one scattering center in a box
- An exact time dependent solution for the unitary quantum gas

PRESENT EXPERIMENTS ON FERMIONS

Typical ENS experimental parameters:

- fermionic ⁶Li atoms: F = 1/2 atomic ground state
- optical trapping, evaporative cooling: $N \sim 10^5 \ k_F \sim 1.6 \times 10^7 \text{m}^{-1} \ k_B T_F \sim 10 \mu \text{K} \ T < 0.2 T_F$
- Why interesting ?
 - strength and sign of interaction tunable with magnetic field
 - scattering length a > 0: a 2-body bound state Bose condensate of dimers
 - scattering length a < 0: Cooper pairs BCS state = condensate of pairs
 - intermediate regime: $a = \pm \infty$ strongly interacting regime $k_F |a| > 1$ stable

WHAT IS A FESHBACH RESONANCE ?

Schematic view:



Low energy scattering properties:

 $B_0 = 820$ Gauss

• scattering length

$$a(B) = a_{bg} \left(1 - \frac{\Delta B}{B - B_0} \right)$$

• Scattering amplitude for $k \times$ true potential range $\ll 1$:

$$f_k \simeq \frac{-1}{-\nu C^{-1} + ik + \hbar^2 k^2 / 2mC}$$

with effective detuning

$$\nu = \epsilon_b(B) + \Delta_b \propto B - B_0 \quad \text{for} \quad B \to B_0$$

and C > 0 coupling intensity

• Low k general scattering theory:

$$f_k = rac{-1}{a^{-1} + ik - rac{1}{2}k^2r_e + \dots}$$

gives

$$a=-rac{C}{
u}$$
 $r_e=-rac{\hbar^2}{mC}<0$

where r_e is effective range.

THE DILUTE GAS REGIME

Crucial assumption: gas dilute at the scale of r_e :

 $|r_e| \ll |a|, k_F^{-1}.$

 \rightarrow zero range model potential possible interactions characterized by a only

Talk of Dima Petrov: regime of gas with effective long range interaction is possible

true range
$$\ll k_F^{-1}, |a| \ll |r_e|$$

WHICH MODEL FOR THE INTERACTION POTENTIAL ?

Requirements for non-perturbative N-body problem:

• hypothesis of thermal equilibrium applicable:

$$\sigma_{1,...,N} \propto e^{-eta H}$$

so that e.g. Quantum Monte Carlo can be used. rules out the 'true' interaction potential

• leads to a well defined mathematical problem! good idea to check on e.g. 2-body problem!

Example of an ill-defined problem:

• The Dirac delta interaction potential in 2D and 3D:

$$V(ec{r_1}-ec{r_2})=g\delta(ec{r_1}-ec{r_2})$$

• 2-body Schrödinger's equation in center of mass frame:

$$E\psi=-rac{\hbar^2}{m}\Delta_{ec{r}}\psi+g\delta(ec{r})\psi(ec{r})$$

• Either $\psi(\vec{r})$ vanishes or diverges in $\vec{r} = \vec{0}$:

$$egin{aligned} &3\mathrm{D}:\Deltarac{-1}{4\pi r}=\delta(ec{r})\ &2\mathrm{D}:\Deltarac{\log r}{2\pi}=\delta(ec{r}). \end{aligned}$$

WHAT IS ψ IN THIS TALK ?

• for spinless bosons:

$$\psi(ec{r_1},\ldots,ec{r_N})=\langleec{r_1},\ldots,ec{r_N}|\psi
angle$$

and is totally symmetric

• for spin 1/2 fermions:

 $\psi(ec{r_1},\ldots,ec{r_N})=\langle+:ec{r_1},\ldots,+:ec{r_n},-:ec{r_{n+1}},\ldots,-:ec{r_N}|\psi
angle$

and is totally antisymmetric with respect to $\vec{r_1}, \ldots, \vec{r_n}$ and with respect to $\vec{r_{n+1}}, \ldots, \vec{r_N}$.

MODEL 1: FERMI PSEUDO-POTENTIAL

Definition:

$$\langle \vec{r_1}, \vec{r_2} | V | \psi
angle = rac{4\pi\hbar^2 a}{m} \delta(\vec{r_1} - \vec{r_2}) \psi_{
m reg}(1=2)$$

where

$$\psi_{\rm reg}(1=2) \equiv \left[\partial_{r_{12}}(r_{12}\psi(\vec{r_1},\vec{r_2}))\right]_{r_{12}\to 0}$$

for fixed center of mass position $\vec{R_{12}}$ of 1 and 2 Basic assumption:

• ψ diverges at most like Green's function

$$\psi(ec{r_1},\ldots,ec{r_N}) = O\left(rac{1}{r_{ij}}
ight) \hspace{0.2cm} orall i
eq j$$

• regularisation operator removes the r_{ij}^{-1} term

MODEL 1: FERMI PSEUDO-POTENTIAL

Advantages:

- Depends only on a
- Ideal for exact analytical calculations:

$$egin{aligned} &(\Delta+k^2)\psi(ec{r}\,)=4\pi a\psi_{
m reg}\delta(ec{r}\,) \ &\psi(ec{r}\,)=\psi_0(ec{r}\,)+4\pi a\psi_{
m reg}G(r) \end{aligned}$$

where ψ_0 solves homogeneous equation, G(r) is Green's function

$$G(r) = -rac{\exp(ikr)}{4\pi r}.$$

Resulting unknown is a function of 3 less spatial coordinates:

$$\psi_{\mathrm{reg}} = \psi_{0,\mathrm{reg}} - i k a \psi_{\mathrm{reg}}.$$

MODEL 1: FERMI PSEUDO-POTENTIAL

Disadvantages:

- Not intuitive: 2-body bound state only for a > 0 $\int -\frac{\hbar^2}{2m} \psi^* \Delta \psi$ is not the kinetic energy
- A modified Hilbert space: equivalent to free waves with boundary conditions

$$\psi(\vec{r_1},\ldots,\vec{r_N}) = A(a^{-1} - r_{ij}^{-1}) + o(1)$$

when $r_{ij} \rightarrow 0$ for fixed $\vec{R_{ij}} = (\vec{r_i} + \vec{r_j})/2$.

- Variational calculation more tricky:
 - -fermions: no Hartree-Fock, no BCS
 - -bosons: no Hartree-Fock, no Hartree-Fock-Bogoliubov, no Jastrow ($\psi = [r_{12}r_{13}r_{23}]^{-1} \sim r_{12}^{-3}$ for $\vec{R}_{12} = \vec{r}_3$)

WHEN THREE PARTICLES MEET

Follow general method in free space:

- formal integration of Schrödinger equation relates $\psi(1, 2, 3)$ to $\psi_{\text{reg}}(i = j, k)$ and the Laplacian Green's function
- Fermi or Bose symmetry: only $\psi_{\mathrm{reg}}(1=2,3)$ required
- in the center of mass frame:

$$\psi_{
m reg}(1=2,3)=\psi_{
m reg}(ec{u}=ec{R_{12}}-ec{r_3})$$

• Fermions: when $\vec{u} = \vec{0}$ and $r_{12} \rightarrow 0$:

$$\psi = -rac{a}{r_{12}}\psi_{ ext{reg}}(ec{0}\,) + o(1) ~
ightarrow \psi_{ ext{reg}}(ec{0}\,) = 0.$$

• Bosons: same result using values $\vec{u} \neq \vec{0}$ and requirement of finite $\psi_{\text{reg}}(\vec{0})$.

Never 3 particles at same point in model 1 !

Definition: discrete δ on a lattice

• Spatial coordinates discretized on a grid:

$$ec{r} = \sum_{lpha = x,y,z} n_lpha l ec{e}_lpha$$

- Usual kinetic energy $\hbar^2 k^2/2m$ for wavevector \vec{k} , but $\vec{k} \in \mathbf{D} \equiv [-\pi/l, \pi/l]^3$.
- Interaction potential:

$$V(ec{r_1}-ec{r_2}) = rac{g_0}{l^3} \delta_{ec{r_1},ec{r_2}}$$

 \bullet *l*-dependence in exact state should disappear if

$$k_F l \ll 1.$$

How to choose the coupling constant g_0 ?

• Exact scattering matrix on the grid:

$$T_{
m grid}(E{+}i\eta) = rac{|ec{r}=0
angle \langle ec{r}=0|}{g_0^{-1} - \int_{f D} d^3k (2\pi)^{-3} (E + i\eta - \hbar^2 k^2/m)^{-1}}$$

• Adjust g_0 to have scattering length a on the grid:

$$g_0^{-1} = g^{-1} - \int_{f D} rac{d^3k}{(2\pi)^3} rac{m}{\hbar^2 k^2} \ g_0 = rac{g}{1-2.442 \, a/l}.$$

similar to 'usual' prescription (see e.g. Randeria).

• $l \ll |a|$ gives $g_0 = -5.14 \,\hbar^2 l/m < 0$: not hard sphere but attractive for $|a| = \infty$

Advantages:

- Regular Hilbert space: for fermions, BCS ansatz can be used
- Link with Hubbard Hamiltonian theory possible
- Negative coupling constant $g_0 < 0$:
 - The gas clearly experiences attraction
 - Quantum Monte Carlo possible for fermions: no sign problem

Disadvantages for bosons: 3 particles can be on same site:

• breaks equivalence with model 1: has Efimov states not present in model 1

$$\psi_{
m reg}(1=2,3) \stackrel{!}{ o} \infty ext{ for } ec{r_3} o ec{R_{12}}. \ \psi\left[ec{r_1},ec{r_2},ec{r_3}=rac{1}{2}(ec{r_1}+ec{r_2})
ight] \stackrel{!}{\sim} rac{1}{r_{12}^2} ext{ for } ec{r_{12}} o 0.$$

• breaks usability of thermodynamics: spectrum not bounded from below for $l \rightarrow 0$:

$$E_0 \leq -N rac{2\pi\hbar^2}{2.442ml^2} (N-2.918)$$

as obtained from variational ansatz $|N:\vec{r}=\vec{0}\rangle$.

A NAIVE BUT INSTRUCTIVE MODEL For a given spin \uparrow fermion:

- \bullet effect of nearest \downarrow modeled by scattering center
- effect of other $N/2 1 \downarrow$ modeled by box of size $\sim
 ho^{-1/3}$
- effect of other N/2 1 \uparrow : Fermi statistics, modeled by $\phi = 0$ boundary conditions
- Trick used in Jastrow MC calculations, see Pandharipande: short range correlations crucial for $k_F|a| > 1$



Relating the model to observables of the gas:

• Energy of the gas vs energy in the box:

$$E=rac{1}{2}N\epsilon$$

• Density of the gas vs radius in the box:

$$a=0: \;\; rac{3}{5}N\epsilon_F=rac{1}{2}Nrac{\hbar^2}{m}\left(rac{\pi}{R}
ight)^2 \;\;\;\; k_FR=\sqrt{5/3}\pi_A$$

Solving the one-body problem:

$$-rac{\hbar^2}{m}\Delta\phi=\epsilon\phi~~\partial_r\ln(r\phi)_{r=0}=-rac{1}{a}$$

• Positive energies $\epsilon = \hbar^2 k^2/m$:

$$\phi(r) \propto rac{\sin[k(r-R)]}{r} ~~ ank R = ka$$

• Negative energies $\epsilon = -\hbar^2 \kappa^2 / m$: $\phi(r) \propto \frac{\sinh[k(r-R)]}{r} \quad \tanh \kappa R = \kappa a$

PREDICTIONS OF NAIVE MODEL



PREDICTIONS OF NAIVE MODEL

Ground branch:

- Connecting two interesting regimes:
 - $-k_F a \rightarrow 0^-$: weakly attractive Fermi gas BCS phase in a full *N*-body theory
 - $-k_F a \rightarrow 0^+$: dilute gas of dimens BEC of dimens in a full *N*-body theory
- Is stable. Even in unitary limit. Thanks to Fermi pressure.
- Energy less than the ideal Fermi gas. For $a = \pm \infty$: effective attraction.
- Crucial idea: adiabatic following degenerate Fermi gas → BEC of dimers BEC of dimers → condensate of "Cooper" pairs

Upper branch:

- $k_F a \rightarrow 0^+$: weakly repulsive Fermi gas.
- For bosons: the standard state of BEC's !
- Is metastable. Relaxes to ground branch by three-body collisions:

 $3 \text{ atoms} \rightarrow 1 \text{ dimer} + 1 \text{ atom}$

A second way to produce a BEC of dimers.

EXPERIMENTAL RESULTS AT ENS

Measuring the expansion energy of the gas:

• expansion with fixed *a*:

$$E_{\text{expansion}} = E_{\text{kin}} + E_{\text{inter}}$$

- expansion with a = 0 possible: gives momentum distribution
- Breaking the molecules just before imaging:

$$a > 0 \rightarrow a < 0$$
 then $a = 0$.



A BEC of dimers



$$rac{a_{
m mol}}{a} = 0.56^{+0.3}_{-0.2} ~{
m vs~theory}~ 0.6.$$

Other groups:

- D. Jin, JILA (Boulder, USA), with 40 K
- R. Grimm, Innsbruck, with ⁶Li
- W. Ketterle, MIT (Boston, USA), with ⁶Li
- A condensate of pairs for $k_F|a| > 1$ reported by D. Jin.

MORE DETAILS ON UNITARY LIMIT $|a| = +\infty$

Known properties:

• Universality: depends only on T/T_F

$$E(T=0) = \eta E^{(0)}(T=0)$$

- \bullet Effective attraction: $\eta < 1$ from Hartree-Fock
- Upper bound from BCS (Randeria):

 $\eta < 0.5906\ldots$

• Fixed Node Green's function Monte Carlo with trial Jastrow-BCS wavefunction (Pandharipande):

 $\eta < 0.44 \pm 0.01$



MORE DETAILS ON ADIABATIC FOLLOWING

Evolution of temperature:

• Gas thermally isolated: for slow change of a, isentropic evolution:

$$S(N, T_i, a_i) = S(N, T_f, a_f).$$

• Bose condensate limit:

$$k_F a \ll 1$$
 $k_B T \ll k_B T_c^{(0)} \ll \hbar^2/ma^2.$

For $k_B T > \mu_{mol}$

$$S\simeq 1.8k_BN\left(rac{T}{T_c^{(0)}}
ight)^3$$

• Ideal Fermi gas limit:

$$k_F(-a) \ll 1$$
 $T > T_c^{BCS}$

$$S\simeq k_B N \pi^2 rac{T}{T_F}$$

• Moving from a > 0 to a < 0 can provide cooling.



MORE ABOUT BALLISTIC EXPANSION

- A very common experimental procedure:
 - prepare trapped gas in steady state
 - switch off trapping potential abruptly
 - $\bullet~{\rm gas}~{\rm freely~expands}~{\rm for}~\sim 20~{\rm ms}$
 - laser beam absorption imaging gives integrated density:

$$ext{signal}(x,y) \propto \int dz \,
ho(x,y,z;t)$$

• used as a 'magnification lens': e.g. to reveal a vortex lattice in a BEC (J. Dalibard)

MORE ABOUT BALLISTIC EXPANSION (2)

- Is it a faithfull 'magnifying lens' ?
 - Yes if expanded density can be related to in situ observables
 - A non-trivial problem because of interactions
 - A sufficient condition: existence of scaling relation

$$ho(x,y,z;t) = rac{1}{\prod_lpha \lambda_lpha(t)}
ho_0 \left[rac{x}{\lambda_1(t)},rac{y}{\lambda_2(t)},rac{z}{\lambda_3(t)}
ight].$$

BRIEF HISTORY OF SCALING SOLUTIONS

- For an ideal gas in a harmonic potential
- For the Boltzmann equation in a harmonic isotropic potential: Boltzmann
- For the Gross-Pitaevskii equation in a harmonic trap:
 - in Thomas-Fermi regime: G. Shlyapnikov, E. Surkov, Yu. Kagan (1996), R. Dum, Y. Castin (1996)
 - -in Thomas-Fermi regime for rotating traps: M. Olshanii, P. Storey (2000), Y. Castin, S. Sinha (2001)
 - -in 2D in isotropic trap: G. Shlyapnikov, E. Surkov, Yu. Kagan (1996)
- For superfluid hydrodynamics in a harmonic trap with equation of state $\mu \propto \rho^{\gamma}$: Stringari, Menotti (2002)

- for *N*-body Schrödinger equation of 1D gas of impenetrable bosons in harmonic trap: is formally equivalent to ideal Fermi gas: Girardeau
- For N-body Schrödinger equation in 2D, isotropic harmonic trap, $1/r_{12}^2$ or $\delta(\vec{r_{12}})$ interaction potential: Pitaevskii, Rosch (1997).
- BUT required regularisation breaks scaling invariance: Olshanii, Pricoupenko (2002) so Pitaevskii result applies only to states with no particles at same point

$$\psi(\ldots, \vec{r_i} = \vec{r_j}, \ldots) = 0 \quad \forall i \neq j$$

like Laughlin state.

SCALING SOLUTION FOR THE 3D UNITARY QUANTUM GAS

The problem in an isotropic trap:

• Free Schrödinger equation over domain $r_{ij} \neq 0$:

$$i\hbar\partial_t\psi=\sum_{i=1}^N\left[-rac{\hbar^2}{2m}\Delta_{ec{r_i}}+rac{1}{2}m\omega^2(t)r_i^2
ight]\psi$$

• plus contact conditions:

$$\psi(ec{r_1},\ldots,ec{r_N}) = rac{A(ec{R}_{ij},\{ec{r_k},k
eq i,j\})}{r_{ij}} + o(1).$$

• Initially, stationary state in static trap $\omega = \omega_0$ with energy E.

Ansatz: gauge plus scaling transform:

$$\psi(ec{r_1},\ldots,ec{r_N}) = rac{e^{-i heta(t)}}{\lambda^{3N/2}(t)} \exp\left[rac{im\dot\lambda}{2\hbar\lambda}\sum r_j^2
ight]\psi_0(ec{r_1}/\lambda,\ldots,ec{r_N}/\lambda).$$

- scaling preserves contact conditions
- gauge transform preserves contact conditions:

$$r_i^2 + r_j^2 = 2R_{ij}^2 + rac{1}{2}r_{ij}^2$$

• solves free Schrödinger equation if

$$egin{aligned} \ddot{\lambda} &= rac{\omega_0^2}{\lambda^3} - \omega^2(t)\lambda \ heta(t) &= E \int_0^t rac{d au}{\hbar\lambda^2(au)}. \end{aligned}$$

CONSEQUENCES OF SCALING SOLUTION

- \bullet Linear response: undamped mode of frequency $2\omega_0$
- Existence of lowering operator:

$$L_{-}=-rac{3N}{2}+rac{E}{\hbar\omega_{0}}-\sum_{j=1}^{N}ec{r_{j}}\cdot\partial_{ec{r_{j}}}-rac{m\omega_{0}}{\hbar}\sum_{j=1}^{N}r_{j}^{2}.$$

 $L_{-}|\psi_{0}
angle$ vanishes or has energy $E-2\hbar\omega_{0}$.

• Virial theorem (F. Chevy):

$$E = 2E_{\mathrm{harm}} > 0$$

 \rightarrow spectrum semi-bounded, stability

NB. For isotropic trap hydrodynamic prediction gives same scaling as exact solution. For anisotropic traps experiments in disagreement with hydrodynamics.

CONCLUSION AND PERSPECTIVES

• Crossover from BEC of composite bosons to BCS transition and strongly interacting regime is being studied experimentally with gases of fermionic atoms

A challenge for theorists !

• To come: rotating superfluid Fermi gases, vortices

• To come: fermionic atoms in optical lattices and the Hubbard model