THE UNITARY GAS

OUTLINE:

- I. Simple facts
- II. How to model the interaction
- III. Dynamical scaling invariance in a trap

I. SIMPLE FACTS

WHAT IS THE UNITARY GAS ?

A gas...

• a dilute system with respect to interaction range:

$$nb^3 \ll 1$$

- Scattering amplitude f_k matters rather than V(r)
- ...at unitary limit:
- For relevant relative momentum k, f_k reaches maximal modulus: maximally interacting gas

$$f_k = -rac{1}{ik}$$

• From optical theorem indeed:

$$\operatorname{Im} f_k = k |f_k|^2 \Rightarrow f_k = -\frac{1}{u(k) + ik}, \quad u(k) \text{ real}$$

WHAT THIS IMPLIES FOR AN ATOMIC GAS

S-wave low k expansion of scattering amplitude:

$$u(k)=rac{1}{a}-rac{1}{2}k^2r_e+\dots$$

- $\bullet a$ is scattering length
- r_e is effective range
- . . . assumed negligible for $kb \ll 1$

Unitary gas as a double limit:

(1) zero range limit $kb \ll 1$, $k|r_e| \ll 1$

- (2) infinite scattering length limit: $k|a| \gg 1$
 - If one assumes $k \sim n^{1/3}$ double limit achieved in present experiments on broad Feshbach resonances $(|r_e| \sim b)$.
 - Assumption $k \sim n^{1/3}$ not necessarily true (effective threebody Efimov attraction, bosons or large mass ratio fermions)

CAN ONE HAVE r_e NON ZERO WITH $b \rightarrow 0$

Yes, simple two-channel model of Feshbach resonance:



- \bullet Tune $E_{ ext{mol}}$ to have $|a| = \infty$
- Then effective range

$$r_e=rac{4b}{\pi^{1/2}}-rac{8\pi\hbar^4}{m^2\Lambda^2}$$

WHY IS THE UNITARY GAS FASCINATING ? Universality:

- no parameter left describing the interaction
- eigenenergies E_i depend on \hbar^2/m and on shape of container $U(\vec{r})$: unit of length set by the container!

Spatial scaling invariance:

- Remains unitary if one changes volume of container.
- Not true for fixed finite value of $a: n^{1/3}a$ changes.
- If one applies to container a similarity of factor λ :

$$egin{aligned} E_i &
ightarrow rac{E_i}{\lambda^2} \ \psi_i(ec{X}\,) &
ightarrow rac{\psi_i(ec{X}/\lambda)}{\lambda^{3N/2}} \end{aligned}$$

DIRECT CONSEQUENCES

In harmonic isotropic trap:

$$rac{E_i}{\hbar \omega} = ext{function}_i(N).$$

In free space:

• No bound state can be at unitarity.

In a box at thermodynamic limit:

• Assume that $E_0/N = e_0$, F/N = f are intensive. $e_0(n/\lambda^3) = e_0(n)/\lambda^2 \rightarrow e_0(n) = \eta e_0^{\text{ideal Fermi gas}}(n).$ $f(n/\lambda^3, T/\lambda^2) = f(n, T)/\lambda^2.$

• Taking the derivative in $\lambda = 1$:

$$rac{5}{3}E-\mu N=TS$$
 (Zwerger)

IS THERE UNITARITY IN LOWER DIMENSIONS ? In 1D:

- Tonks-Girardeau Bose gas.
- Mappable to an ideal Fermi gas.

In 2D:

• Low-k scattering characterized by a_{2D} :

$$-rac{1}{f_k} = -\ln(k a_{2D}/2) - \gamma + i \pi/2 + \dots$$

 $\psi_0(r) = \ln(r/a_{2D}) \quad ext{for} \quad r > b.$

- No scale invariance for finite a_{2D} .
- $a_{2D} \rightarrow +\infty$: ideal gas.
- Have $n^{1/2}a_{2D} \sim 1$ to maximize interactions.

IS THERE UNITARITY IN OTHER PARTIAL WAVES ? P-wave interaction for fully polarized fermions:

$$u(k) = rac{1}{k^2 \mathcal{V}_s} + lpha + \dots$$

- Tune \mathcal{V}_s to infinity with Feshbach resonance.
- Can one have $\alpha = 0$ at resonance ?
- Lower bound for compact support potential of radius b:

 $\alpha_{\rm res}b \geq 1.$ (Pricoupenko)

 \bullet For \mathcal{V}_s large and negative, $|u(k)| \ll k$ around

$$k_0 = rac{1}{\sqrt{lpha |\mathcal{V}_s|}}.$$

IS THE UNITARY GAS ATTRACTIVE OR REPULSIVE ?

- **Common sayings:**
 - a > 0: effective repulsive interaction.
 - a < 0: effective attractive interaction.
 - $|a| = \infty$: gas properties do not depend on the sign of a.

Naive way out of this paradox: (Kokkelmans)

- ullet mean field with k-dependent coupling constant $-{
 m Re}\,f_k$
- unitary gas would then be non-interacting.

IS THE UNITARY GAS ATTRACTIVE OR REPULSIVE ? Answer to paradox in short:

- Start from weakly interacting gas.
- Two adiabatic procedures

$$a = 0^+ \rightarrow a = +\infty$$
 and $a = 0^- \rightarrow a = -\infty$

lead to different states, that is they follow different branches. Illustration on a toy model for fermions(Pricoupenko, Castin):

 \bullet A matter wave in hard wall spherical cavity of radius ${\pmb R}$

$$\phi(R)=0 \qquad R\sim n^{-1/3}$$

to mimick Pauli exclusion principle.

• In presence of a scattering center at the origin:

$$\phi(r)=A\left(rac{1}{r}-rac{1}{a}
ight)+o(1).$$

to mimick nearest neighbour interaction.

THE LOWEST ENERGY BRANCHES OF TOY MODEL



II. HOW TO MODEL THE INTERACTION

APPROACH 1

- A finite range model:
 - \bullet potential with finite range b and infinite a
 - calculate eigenenergies, thermodynamic properties, ...
 - go to b = 0 limit at the end of the calculation
- Non-trivial question: universality
 - Eigenstate universal, i.e. reaches unitary limit, if (E_i, ψ_i) converge for $b \to 0$.
 - Typical non-universal state: $E_i \to -\infty$
 - To use $\rho = \exp(-\beta H)$, avoid models with non-universal states: negative V(r) not good for large N (Seiringer, Lobo)
 - Favor models solvable by Quantum Monte Carlo.

APPROACH 2

Replace interaction by Bethe-Peierls contact conditions:

• Hamiltonian is the one of the ideal gas

$$H=-rac{\hbar^2}{2m}\Delta_{ec{X}}+rac{1}{2}m\omega^2X^2$$

- The domain D(H) is not the ideal gas one!
- Contact cond. for $r_{ij} \to 0$ at fixed centroid $\vec{R}_{ij} \neq \vec{r}_k$: $\psi(\vec{X}) = A_{ij}(\vec{R}_{ij}; \{\vec{r}_k, k \neq i, j\}) \left[\frac{1}{r_{ij}} - \frac{1}{a}\right] + o(1)$
- Scale invariance of D(H) to ensure universality if $\psi \in D(H), \psi_{\lambda} \in D(H) \forall \lambda > 0$ with $\psi_{\lambda}(\vec{X}) = \psi(\vec{X}/\lambda)$.
- NB. Here we exclude $\vec{r}_i = \vec{r}_j$. Otherwise a regularized delta interaction pseudo-potential appears.

REMINDER: DOMAIN OF A HAMILTONIAN

Practical definition:

- D(H) is the set of wave functions over which the action of Hamiltonian is represented by differential operator H.
- If one does not care, paradoxes ... due to errors. Simple example:
 - One particle in 1D in a box:

$$H=-rac{1}{2}rac{d^2}{dx^2}$$
 .

with boundary conditions $\psi(0) = \psi(1) = 0$.

• A wavefunction in the domain:

$$egin{aligned} \psi(x) &= x(1-x).\ \langle H
angle_\psi &= 5 \ ; \ \langle H^2
angle_\psi &= 0?. \end{aligned}$$

This last result is wrong: $H\psi \notin D(H)$. Right value: 30.

NON-TRIVIAL QUESTION IN APPROACH 2

Is the Hamiltonian self-adjoint ?

- This amounts to proving the unitarity of the gas.
- For N = 2: answer is yes. (book by Albeverio)
- For N = 3 bosons: no. See later.
- For N = 3 equal mass fermions: probably yes.
- For $N \ge 4$ equal mass fermions: ?

Partial universality:

- Restrict H to subspace where it is hermitian.
- This means: A non-complete family of universal states.
- For N = 3 bosons: all universal states determined. See later. (Jonsell, Heiselberg and Pethick; Werner and Castin)

• For arbitrary number N of bosons, trivial universal states (common to ideal gas) with $A_{ij} \equiv 0$:

$$\psi(ec{X}) o 0 \quad ext{for} \quad r_{ij} o 0.$$

• These trivial states dominate the ideal gas density of states at high energy. (Werner and Castin)

A TRIVIAL QUESTION IN APPROACH 2

I see no interaction energy in H, is the energy of kinetic nature only ?

Answer: no.

$$egin{aligned} E_{ ext{kin}} &= \int rac{\hbar^2}{2m} |\partial_{ec{X}} \psi|^2 = +\infty. \ E_{ ext{kin}} + E_{ ext{int}} &= -\int rac{\hbar^2}{2m} \psi^* \Delta_{ec{X}} \psi. \end{aligned}$$

OUR CANDIDATE FOR APPROACH 1

A Hubbard-type lattice model (here for spin 1/2 fermions):

- cubic lattice of step b.
- "tunneling": one-body eigenstates are plane waves with dispersion relation ϵ_k

$$ec{k} \in \mathcal{D} \equiv \left[-rac{\pi}{b}, rac{\pi}{b}
ight]^3 \hspace{0.5cm} ext{and} \hspace{0.5cm} \epsilon_k = rac{\hbar^2 k^2}{2m}$$

ullet on-site interaction with coupling constant g_0

$$H = \sum_{ec{k} \in \mathcal{D}} \sum_{\sigma=\uparrow,\downarrow} \epsilon_k a^\dagger_{ec{k},\sigma} a_{ec{k},\sigma} + g_0 \sum_{ec{r}} b^3 \hat{\psi}^\dagger_\uparrow(ec{r}) \hat{\psi}^\dagger_\downarrow(ec{r}) \hat{\psi}_\downarrow(ec{r}) \hat{\psi}_\downarrow(ec{r})$$

• Field commutation relations mimicking continuous space ones:

$$\{\hat{\psi}_{\sigma}(\vec{r}\,),\hat{\psi}^{\dagger}_{\sigma'}(\vec{r}\,')\} = \delta_{\sigma\sigma'}rac{\delta_{\vec{r},\vec{r}\,'}}{b^3}.$$

HOW TO CHOOSE THE COUPLING CONSTANT g_0

To have the correct scattering length: (Mora, Castin)

- scattering of two particles in the infinite lattice
- for a zero total momentum:

$$H_{
m rel}=rac{p^2}{m}+V \quad {
m with} \quad V=g_0ert ec r=ec 0\,
angle \langle ec r=ec 0\, ert$$

• calculate the T-matrix on the grid

$$T(E + i0^{+}) = V + VG_{rel}(E + i0^{+})V$$

• expand at low energy, setting $E = \hbar^2 q^2/m, \ q \ge 0$: $\langle \vec{k} \, | T(E+i0^+) | \vec{k} \,'
angle = rac{4\pi \hbar^2/m}{a^{-1} + iq + O(q^2b)}$ HOW TO CHOOSE THE COUPLING CONSTANT g_0 (2) Result and discussion:

$$g_0 = rac{4\pi \hbar^2 a/m}{1-Ca/b} \quad ext{with} \quad C = 2.442\ 749\dots$$

- Born regime: $|a| \ll b$
- ullet impenetrable regime: $g_0 = +\infty$ gives a = b/C
- infinite scattering length:

$$g_0=-rac{4\pi\hbar^2 b}{C}$$

0

so an attractive Hubbard-type model with $g_0 \rightarrow 0^-$ in unitary limit.

ADVANTAGES OF THIS LATTICE MODEL For fermions, link with condensed matter physics:

• Unitary limit = zero filling factor limit of Hubbard model with

$$rac{U}{J}=rac{g_0/b^3}{\hbar^2/(2mb^2)}= ext{well chosen constant}$$

- Quantum Monte Carlo possible with no sign problem: $T_c^{\text{Svistunov}} \simeq 0.15T_F$ $T_c^{\text{Bulgac}} \simeq 0.2T_F$ $\eta \simeq 0.44$ and gap $\Delta \simeq 0.44E_F$ (Juillet) From a theoretical point of view:
- no tricky D(H), standard variational methods apply:

$$\eta \leq \eta_{\rm BCS} = 0.5906...$$
 (Randeria)

From an experimental point of view in a lattice:

• For bosons: $|a| = \infty$ without a Feshbach resonance

 $b \rightarrow 0$ LATTICE MODEL \iff BETHE-PEIERLS ? (Pricoupenko, Castin)

Case of two particles:

• Proof of equivalence for the eigenergies E_i

Case of three equal mass fermions:

- numerically, coincidence.
- analytically: if finite limit of $E_i(b)$ exists, coincidence.
- all $E_i > 0$ checked up to b/L = 1/81 (diagonalisation of a matrix 531 441 \times 531 441)

THE TWO MODELS FOR 3 EQUAL MASS FERMIONS



CASES OF $b \rightarrow 0$ LATTICE MODEL \neq BETHE-PEIERLS Case of $|a| = \infty$ bosons:

ullet Variational calculation with $|N:ec{r}=ec{0}
angle$

$$E_0(b) \leq g_0 N[N-2.92]/(2b^3) \stackrel{b
ightarrow 0}{
ightarrow} -\infty.$$

- Approaches 1 and 2 are then not equivalent.
- Same result for 2 massive fermions and a light particle:
 - Variational calculation with the 2 fermions localized on neighboring sites:

$$E_0(b) \leq -0.2 rac{\hbar^2}{mb^2} \left(1-42 rac{m}{M}
ight)$$

• For a large enough mass ratio M/m, Pauli principle not sufficient to prevent 3-body deeply bound states (see lecture by Petrov).

III. DYNAMICAL SCALING INVARIANCE IN A TRAP

FIRST MOMENT OF THE TRAPPING ENERGY: VIRIAL THEOREM

We consider a normalized eigenstate of H:

$$H\psi=E\psi$$

then one has the virial theorem: (exp. check: Thomas)

$$\langle \psi | H | \psi
angle = 2 \langle \psi | H_{ ext{trap}} | \psi
angle$$

with $H_{ ext{trap}} = rac{1}{2}m\omega^2 X^2.$

Proof: for a Hermitian H, an eigenstate is a stationary point of the mean energy

$$E(\lambda)\equiv rac{\langle\psi_\lambda|H|\psi_\lambda
angle}{\langle\psi_\lambda|\psi_\lambda
angle}=\lambda^{-2}\langle\psi|H{-}H_{
m trap}|\psi
angle{+}\lambda^2\langle\psi|H_{
m trap}|\psi
angle.$$

$$\left(rac{dE}{d\lambda}
ight) (\lambda=1)=0.$$

SCALING SOLUTION IN A TIME DEPENDENT TRAP Isotropic trap is time dependent for t > 0:

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

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

• plus contact conditions for $r_{ij} \rightarrow 0$:

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

- Initially, stationary state in static trap $\omega(t=0)=\omega$ with energy E_{\cdot}
- Relevant for experiments: time of flight, collective modes.

Ansatz: gauge plus scaling transform:

$$\psi(ec{X},t) = rac{e^{-i heta(t)}}{\lambda^{3N/2}(t)} \exp\left[rac{im\dot{\lambda}}{2\hbar\lambda}X^2
ight]\psi(ec{X}/\lambda(t),0).$$

• 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 Schrödinger equation if

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

Y. Castin, Comptes Rendus Physique 5, 407 (2004).

PRACTICAL INTEREST OF SCALING SOLUTION Ballistic expansion is a perfect lens:

- For mean density $n(\vec{r},t) = rac{1}{\lambda^3(t)} n_0[\vec{r}/\lambda(t)]$
- but also for higher order density correlation functions:

$$g^{(2)}(ec{r_1},ec{r_2},t) = rac{1}{\lambda^6(t)} g_0^{(2)}[ec{r_1}/\lambda(t),ec{r_2}/\lambda(t)].$$

- Applies even at $T > T_c$ and for all gas polarisations.
- But requires $|a| = \infty$ and an isotropic harmonic trap.

Can one relax these two conditions ?

- At first sight, no:
 - -finite |a| breaks scaling invariance.
 - -anisotropic trap expected to lead to anisotropic expansion, but anisotropic scaling does not preserve D(H)

• However there is a clever way to lift the two conditions (Lobo).

APPLICATION: RAISING/LOWERING OPERATORS

Gedanken experiment: weak change of ω for $0 < t < t_f$:

• Resulting change for the scaling parameter:

$$\lambda(t) - 1 = \epsilon \ e^{-2i\omega t} + \epsilon^* \ e^{2i\omega t} + O(\epsilon^2).$$

An undamped mode of frequency 2ω (Pitaevskii, Rosch).

• Resulting change for the wavefunction:

$$egin{aligned} \psi(ec{X},t) &= \left[e^{-iEt/\hbar} - \epsilon e^{-i(E+2\hbar\omega)t/\hbar}L_+
ight. \ &+ \epsilon^* e^{-i(E-2\hbar\omega)t/\hbar}L_-
ight] \psi(ec{X},0) + O(\epsilon^2) \end{aligned}$$

• Raising and lowering operators:

$$L_{\pm} = \pm \left[rac{3N}{2} + ec{X} \cdot \partial_{ec{X}}
ight] + rac{H}{\hbar \omega} - m \omega X^2/\hbar$$

• Repeated action of L_{\pm} : ladder of eigenenergies with equal spacing $2\hbar\omega$.

LINK WITH SO(2,1) LIE ALGEBRA (Pitaevskii, Rosch) Trapped unitary gas has SO(2,1) hidden symmetry:

- Energy ladders directly from commutation relations: $[H,L_{\pm}] = \pm 2\hbar\omega\,L_{\pm}$ $[L_{+},L_{-}] = -4H/(\hbar\omega)$
- Do not forget to check that L_{\pm} preserve domain.
- Introduce what will be the generators of the group:

$$T_1\pm iT_2=rac{L_\pm}{2} \qquad T_3=rac{H}{2\hbar\omega}$$

• Then commutation relations of SO(2,1) Lie algebra:

$$[T_1, T_2] = -iT_3$$
 $[T_2, T_3] = iT_1$ $[T_3, T_1] = iT_2$

• Casimir operator, which commutes will all the elements of the algebra

$$C = -4 \left[T_1^2 + T_2^2 - T_3^2 \right] = H^2 - (\hbar \omega)^2 (L_+ L_- + L_- L_+)/2$$

EXISTENCE OF A BOSONIC DEGREE OF FREEDOM Key point: the ladders are semi-infinite

• Virial theorem: $E \geq 3\hbar\omega/2$. Action of L_{\perp} terminates:

$$L_-\psi_g=0,$$

so one can define the ground energy step operator H_{g} .

• In terms of Casimir operator:

- $ullet {f From SO(2,1) algebra to creation/annihilation operators} \ b = [2(H+H_g)/\hbar\omega]^{-1/2}L_-, \ \ b^\dagger = L_+[2(H+H_g)/\hbar\omega]^{-1/2} \ [b,b^\dagger] = 1.$
- Unitary gas has a decoupled bosonic degree of freedom, the breathing mode:

$$H=H_g+2\hbar\omega b^\dagger b \quad {
m with} \quad [b,H_g]=0.$$

SECOND MOMENT OF THE TRAPPING ENERGY

In principle, fluctuations of trapping energy $H_{\rm trap} = m\omega^2 X^2/2$ are measurable:

• At thermal equilibrium in canonical ensemble:

$$4\langle H_{
m trap}^2
angle = \langle H^2
angle + \langle H
angle \hbar \omega \left[2\langle b^\dagger b
angle + 1
ight].$$

• Proof:

$$egin{aligned} H_{ ext{trap}} &= rac{1}{2} H - rac{\hbar \omega}{4} \left(L_+ + L_-
ight) \ H_{ ext{trap}} &= rac{\hbar \omega}{2} A^\dagger A \quad ext{with} \quad A = \left[rac{H_g}{\hbar \omega} + b^\dagger b
ight]^{1/2} - b. \ \langle H_g \, b^\dagger b
angle &= \langle H_g
angle \langle b^\dagger b
angle. \end{aligned}$$

• Thermometry: measuring fluctuations of the breathing mode of the unitary gas

SEPARABILITY IN HYPERSPHERICAL COORDINATES

• Hyperspherical coordinates $(X, \vec{n} \equiv \vec{X}/X)$

• Integrate
$$L_-\psi_g=0$$
:

 $[3N/2+X\partial_X+E_g/(\hbar\omega)-m\omega X^2/\hbar]\psi_g(ec X)=0.$

$$\psi_g(ec{X}\,)=e^{-m\omega X^2/2\hbar}\,X^{E_g/(\hbar\omega)-3N/2}f(ec{n}).$$

- Mapping to scale invariant zero energy free space eigenstates (Tan)
- Gives excited ladders in terms of Laguerre polynomials.
- The hyperangular problem was solved by Efimov for N=3 .
- This gives the solution to the trapped 3-body unitary problem (Werner, Castin).

MORE DETAILS ON SEPARABILITY FOR N > 2Form of the N-body wavefunction:

$$\psi(\vec{X}) = \psi_{CM}(\vec{C})\phi(\vec{\Omega})R^{(5-3N)/2}F(R)$$

- ullet uses separability of the center of mass $ar{C}$
- uses separability in internal spherical coordinates $(R, \vec{\Omega})$
- contact conditions put a constraint on $\phi(\vec{\Omega})$ only, for Laplacian on unit sphere of dimension 3N 4:

$$\Delta_{ec\Omega} \phi = -\Lambda \phi.$$

• Effective 2D Schrödinger equation for the radial part:

$$egin{aligned} &-rac{\hbar^2}{2m}\Delta_{2D}F(R)\!+\!\left(\!rac{\hbar^2s^2}{2mR^2}\!+\!rac{1}{2}m\omega^2R^2\!
ight)F(R) = E_{
m int}F(R) \ & ext{with}\ s^2 = \Lambda + [(3N-5)/2]^2. \end{aligned}$$

PHYSICAL DISCUSSION FOR N = 3

$$-rac{\hbar^2}{2m}\Delta_{2D}F(R)+\left(rac{\hbar^2s^2}{2mR^2}+rac{1}{2}m\omega^2R^2
ight)F(R)=E_{
m int}F(R)$$

Efimov: *s* is a root of transcendental equations. A good case: equal mass fermions

- Proof that all $s^2 \ge 0$. (Werner and Castin)
- Then one chooses $s \ge 0$. Numerically s > 1.
- ullet Spectrum $E=(s+1+2q)\hbar\omega,\,q\in\mathbb{N}.$
- A bad case: bosons
 - There is a negative s^2 : $s_0 = i \times 1.00624...$ then Whittaker functions are square integrable solutions $\forall E_{\text{int}} \in \mathbb{R}$: Hamiltonian not hermitian.
 - Proof that all other s^2 are ≥ 0 . (Werner and Castin)

SUGGESTIONS OF EXPERIMENTS

- For fermions:
 - measure gap Δ
 - \bullet check/use of scaling transform: breathing mode, measure $g^{(2)}$
 - mixture of fermions with different masses
- For bosons:
 - 3-body universal states for $|a| = \infty$ at the node of an optical lattice
 - $|a| = \infty$ bosons in an optical lattice far from a Feshbach resonance.