VIJAY
and
CONDENSED MATTER PHYSICS

(esp. cold atoms)

Tony Leggett
UIUC

"Celebrating Vijay Pandharipande"

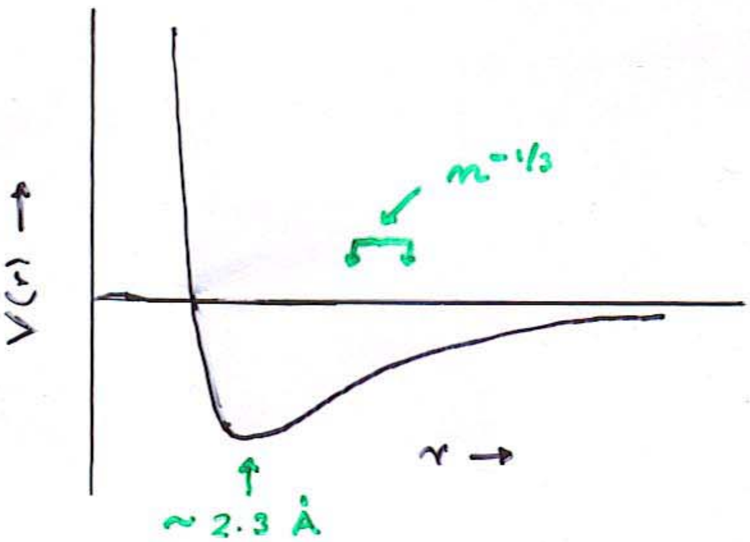
30 Sept. 2006

LIQUID HE

He atom closed-shell, always in electronic groundstate. ^{4}He, $I = 0$ (boson), ^{3}He, $I = 1/2$ (fermion)

nuclear spin

interatomic potential approx. vdW:



no 2-p bound state for 3-3 or 3-4, prob. v. weakly bound state for 4-4.

important work of Vijay and collaborators inter alia on

- single-particle spectrum of ^{3}He
- droplets of liq. ^{4}He and ^{3}He
- condensate fraction + mom^m distr^n of ^{4}He
- $S(q\omega)$ of ^{4}He

.....

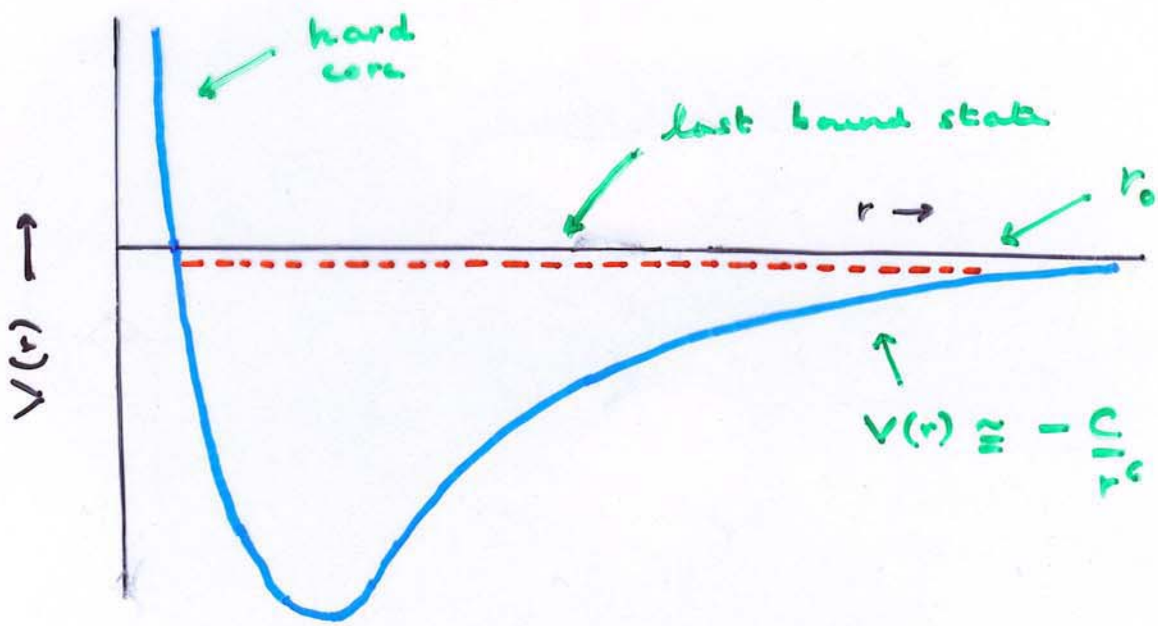
DILUTE ALKALI GASES : THE SYSTEMS

^{87}Rb, ^{23}Na, ^{7}Li, ^{1}H } bosons

^{40}K, ^{6}Li } fermions

electronic groundstate: $L = 0$, $S = 1/2$, $\underset{\text{nuc. spin}}{I} \neq 0$

so hyperfine-split (eg ^{40}K: $F = 9/2$ or $7/2$) : but, in expt. can stabilize single HF species, or pair.



$r_0 \equiv (mC/\hbar^2)^{1/4} \sim 50\text{-}100$ Å

interparticle separation $\gtrsim 10^4$ Å $\Rightarrow nr_0^3 \ll 1$

for $k_BT \ll \hbar^2/mr_0^2 \sim 100\,\mu K$ can neglect scattering in $l \neq 0$ partial waves, so:

VERY DILUTE GAS, S-WAVE SCATTERING

Dilute Gas, s-wave Scattering (only)

$$\Psi(r_1 r_2 \dots r_i \dots r_j \dots r_N) \equiv \Psi(\dots, \overbrace{|\underset{\sim}{r}_i - \underset{\sim}{r}_j|}^{r_{ij}})$$

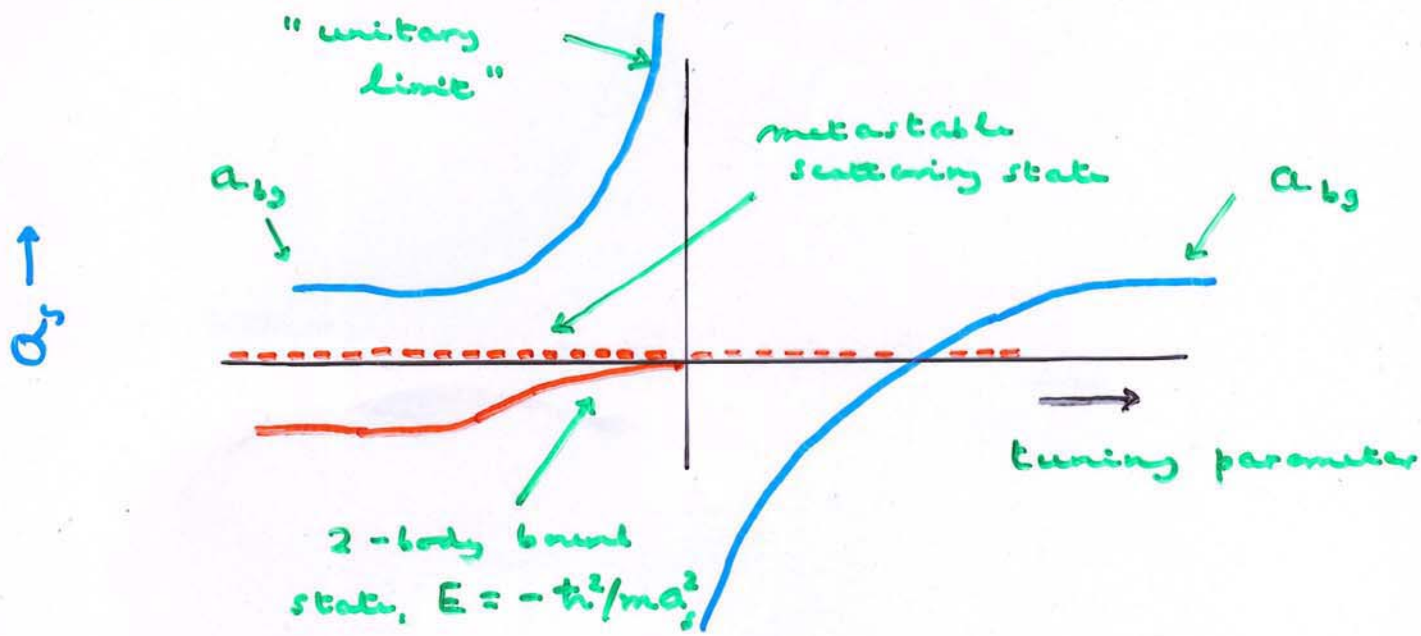
$$\sim \text{const.} \left(1 - \frac{a_s}{r_{ij}}\right) \qquad (r_0 \ll r_{ij} \ll n^{-1/3})$$

s-wave scattering length

typically, $a_s \sim r_0 \sim 50-100$ Å

but, by using Feshbach resonance, can tune a_s to arb. large +ve/−ve value. Mostly "single-channel"

Behavior near resonance (2-body problem)



Many-body problem:

bosons: $a_s < 0$ unstable

but can study metastable $a_s > 0$ state

fermions: both signs of a_s stable.

Dilute Bose Gas with Repulsion $(a_s > 0)$

$(T = 0)$.

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m} \nabla_i^2$$

with boundary cond^n:

$$\Psi_N \sim \text{const.}\left(1 - \frac{a_s}{r_{ij}}\right)$$

for $r_0 \ll r_{ij} \ll n^{-1/3}$

(nb. $n r_0^3 \ll 1$ always)

Known results:

(a) $a_s = 0$ (free gas)

GS energy $\rightarrow E/N = 0$, $N_0 = N$ condensate number

(b) weak repulsion, $n a_s^3 \ll 1$:

$$E/N = \frac{2\pi\hbar^2 n a_s}{m}\left(1 + o(n a_s^3)^{1/2} + \ldots\right)$$

$$N_0/N = 1 - o(n a_s^3)^{1/2} + \ldots \qquad \text{(Lee, Yang 1957)}$$

What happens for $n a_s^3 \gtrsim 1$?

In limit $n a_s^3 \gg 1$, b.c. becomes simply $\Psi_N \sim r_{ij}^{-1}$, so a_s drops out + only characteristic length is $n^{-1/3}$.

$\Rightarrow$ expect in this limit,

$$E/N = (n^{2/3}\hbar^2/m)\cdot A \qquad A = ?$$

$\uparrow$: variational calculations generally fail for this problem, because the "groundstate" we are seeking is metastable with respect to formation of molecules.

S. Cowell, H. Heiselberg, I.E. Mazets, J. Morales, VRP and C.J. Pethick, PRL $\underline{88}$, 210403 (2002)

Jastrow ansatz: $\Psi_N(r_1 r_2 \ldots r_N) = \prod_{i<j} f(\underset{\sim}{r}_i - \underset{\sim}{r}_j)$

Determine $f(r_{ij}) \equiv \psi(r_{ij})/r_{ij}$ by LOCV method:

"lowest order constrained variational"

$$-\frac{\hbar^2}{m}\frac{d^2\psi}{dr^2} = \lambda\psi$$

with b.c's:

(a) $\lim_{r\to 0} \psi'/\psi = -a_s^{-1}$

(b) beyond some "healing distance" $d \sim n^{-1/3}$, $f(r) = 1$, and $f'(r) = 0$ at $r = d$.

(i.e. $\psi'/\psi = d^{-1}$)

With these conditions

$$\psi(r) = \text{const.}\ \sin k(r-b)$$

where k and b are fixed by

$$\frac{(kd)^{-1}\tan kd - 1}{1 + (kd)\tan(kd)} = \frac{a_s}{d}$$

$$b = \tan^{-1}(ka_s)/k$$

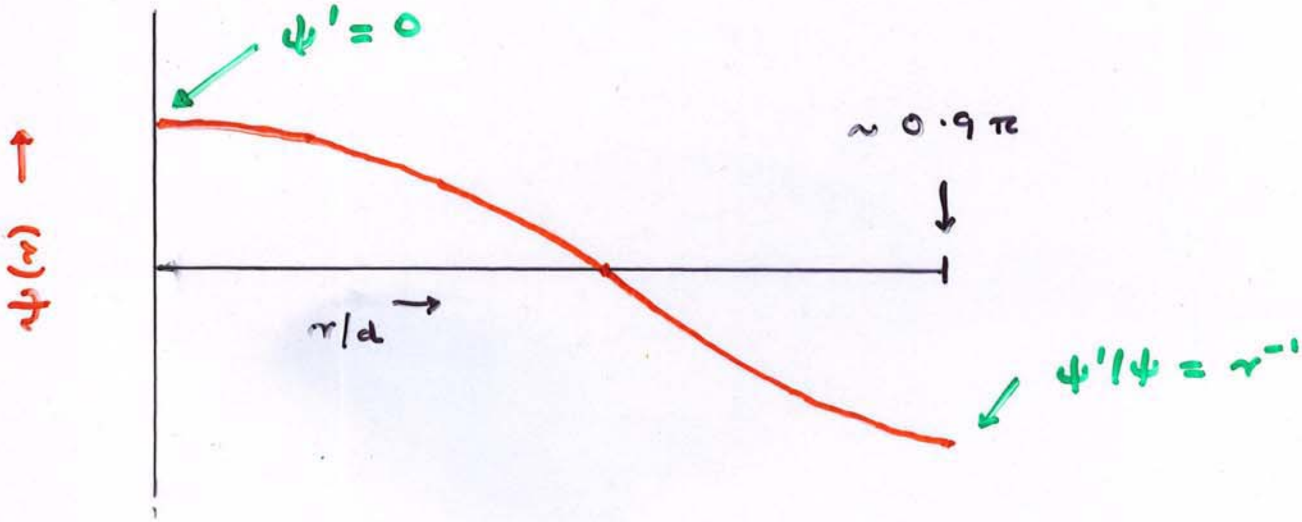
d is fixed by

$$4\pi\int_0^d |\psi(r)|^2\, dr = n^{-1}$$

and

$$E/N = \hbar^2 k^2/2m.$$

Result in unitary limit ($a_s \to \infty$):



$A = 13.33$

Cowell et al. also calculate E/N for finite a_s: agree with Lenz (GP) formula in dilute limit, close to hard-sphere results for $na_s^3 \lesssim 1$.

Also calculate N_0/N and find it vanishes for $a/n^{-1/3} \gtrsim 1.2$. (note not expected to apply in hard-sphere or ^{4}He-like case, in absence of phase transition).

THE "BCS-BEC CROSSOVER" PROBLEM

System: 2 different species of fermions, very dilute gas ($nr_0^3 \ll 1$), attractive interaction.

(Expt: ^{6}Li, ^{40}K)

Characteristic dimensionless parameter:

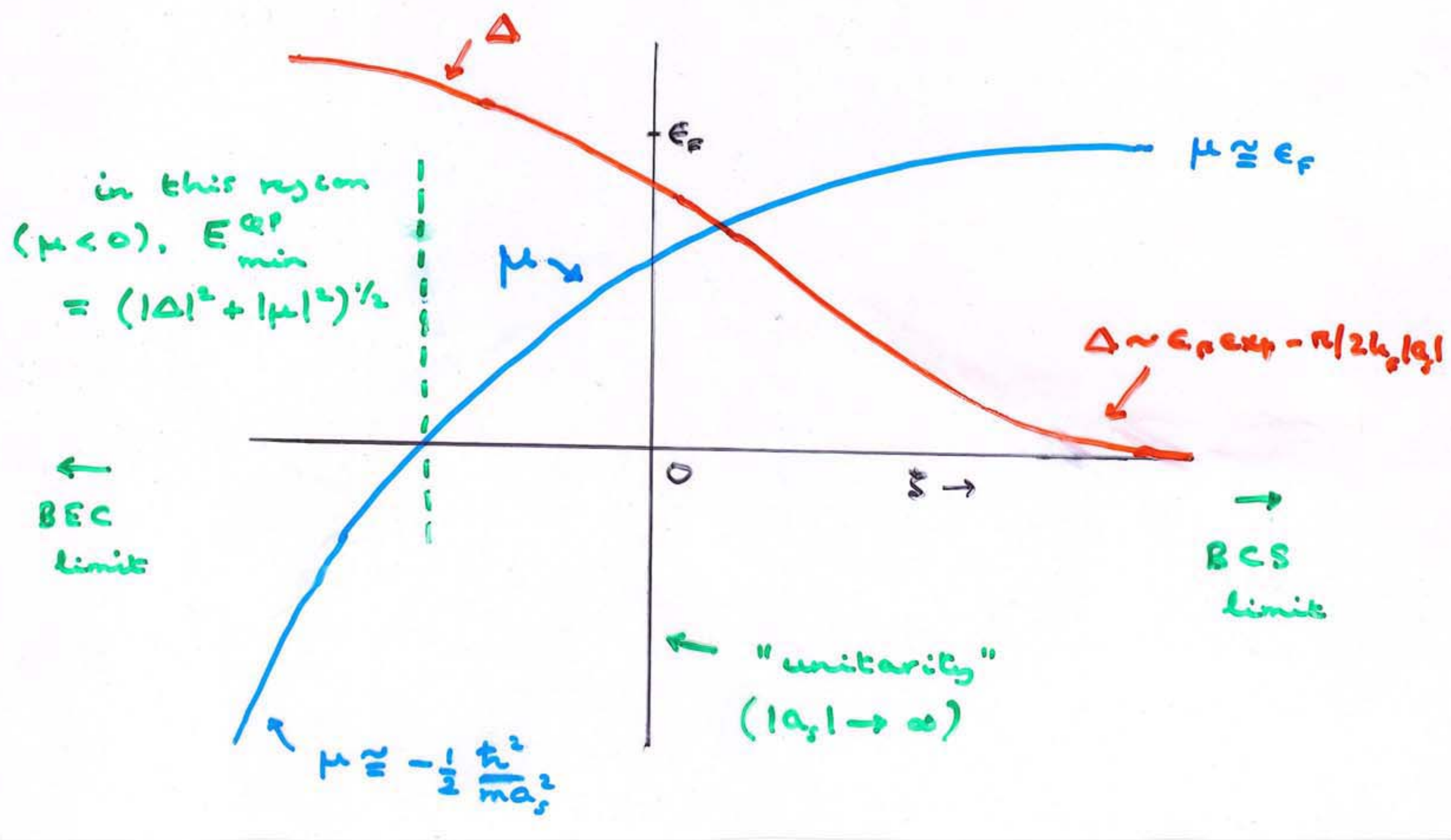
$$na_s^3 \rightarrow -1/k_F a_s \equiv \zeta \qquad (n = k_F^3/3\pi)$$

What do we expect? ($T=0$)

(a) $\zeta \rightarrow +\infty$ (a_s −ve + small): BCS limit, expect Cooper pairing, $\Delta \sim \epsilon_F \exp - \pi/2k_F|a_s|$

(b) $\zeta \rightarrow -\infty$ (a_s +ve + small): limit of tightly bound molecules, expect Bose condensate of them.

Obvious conjecture:



The problem: N fermions, equal nos. ↑ and ↓, $N_{tot} = (k_F^3/3\pi^2)$

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2$$

subject to b.c.

$$\Psi_N \sim \text{const.}(1 - a_s/r_{ij})$$ for antiparallel-spin particles i, j

(in dilute limit, parallel-spin particles noninteracting)

"NAIVE" ANSATZ (Eagles 1969, AJL 1980, Randeria et al. 1985, Strinati et al. 2005 ...): BCS!

$$\Psi_N = \mathcal{N} \cdot \mathcal{A} \cdot \{\varphi(r_1 - r_2 : \sigma_1\sigma_2)\,\varphi(r_3 - r_4 : \sigma_3\sigma_4) \ldots \varphi(r_{N-1} - r_N : \sigma_{N-1}\sigma_N)\}$$

$\langle\Psi_N|\hat{H}|\Psi_N\rangle =$:

(1) pairing terms ← fully taken into account

(2) Fock " ← vanish in dilute limit

(3) Hartree " ← ??

equivalently: each term of $\Psi_N^{(naive)}$ satisfies b.c. for paired particles only, e.g. 1st term satisfies it for 1, 2 but not (eg) for 1, 3.

Output of main ansatz: (calcn: analytic except for 2 1D numerical integrals)

$\mu(S)$, $\Delta(S)$

hence also $(E/N)(S)$.

Vijay's work:

J. Carlson, S-Y. Chang, VRP, KE Schmidt, PRL 91, 050401 (2003)

" ⇆ " " Phys. Rev. A 70, 043602 (04)

S.Y. Chang and VRP, PRL 95, 080402 (05)

" " Phys. Rev. B 73, 212502 (06)

NB.: In this case we seek the stable groundstate, so direct variational calculation should work.

(but optimal from different!)

Ansatz: $\Psi_N = \prod_{\substack{ij \\ (j>i)}} f(r_{ij})\, \Psi_{BCS}\{r_i, \sigma_i\}$

Jastrow   BCS (as in naive ansatz)

Variational technique: GFMC (Green's function Monte Carlo)

N (~20-40) particles in box.

Output: (as $f(\xi)$) $(\xi \equiv -(k_F a_s)^{-1})$

E/N, Δ, pair wf ...

at unitarity ($|a_s| \to \infty$):

$E/N = 0.44\, E_{FG}$ (naive: $0.59\, E_{FG}$)

$\Delta = 0.99\, E_{FG}$ " 1.13 "

"naive" theory better for Δ than for E/N.

Groundstate energy at unitarity as fraction of free-gas value ($\frac{3}{5} N \epsilon_F$):

Vijay et al.: 0.44 naive: 0.59

expt:

Innsbruck 04:	0.32 ± 0.12
ENS 04:	0.36 ± 0.15
Duke 05:	0.51 ± 0.04
Rice 06:	0.46 ± 0.05

(Some) Open Questions

1. General:

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2$$

$$\Psi_N(r_1 r_2 \dots r_N) \sim r_{ij}^{-1} \quad \text{for } r_{ij} \to 0$$

analytically soluble ??

2. Bose case:

(a) $T = 0$: does $\rho_s \to 0$ smoothly at some (na_s^3)?

(b) $T \neq 0$: rigorous limits on T_c?

failing that, on $N_0(T) / \rho_s(T)$?

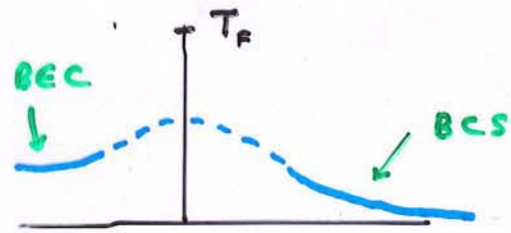
3. Fermi case:

(a) stable groundstate:

many experiments measure quantities not traditionally (much) addressed by theorists (eg N_0)

(b) $T_c(\xi)$?

(c) kinetics



(d) repulsive a_s,

metastable case

(e) unequal spin populations

.....