Small droplets made of ^{3}He and ^{4}He atoms

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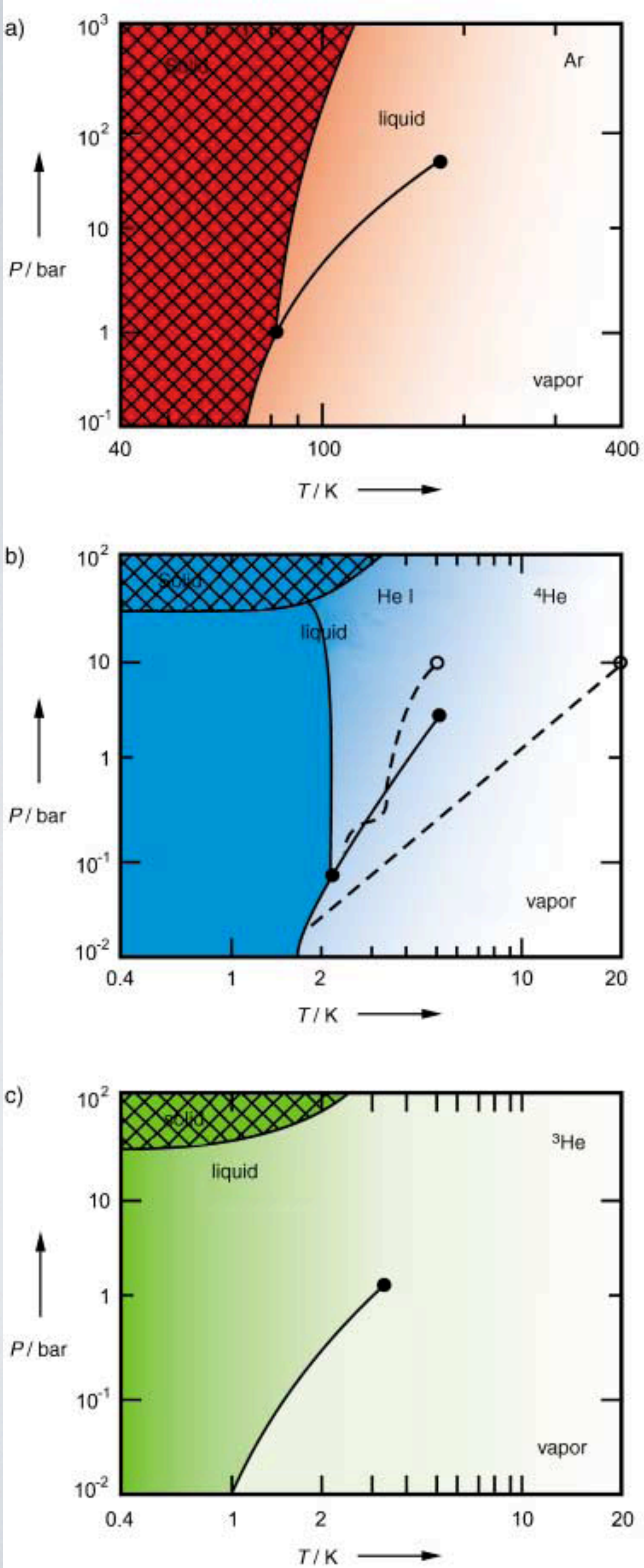
"Spin-offs" of the Strasbourg-Madrid Shell-Model collaboration

1 - M. Barranco, J.N., A. Poves:
Structure and stability of ^{3}He droplets, Phys. Rev. Lett. **78**, 4729 (1997)
2 - J. N., A. Poves, M. Barranco, M. Pi:
Shell structure in mixed ^{3}He-^{4}He droplets, Phys. Rev. A **69**, 023202 (2004)
3 - S. Fantoni, R. Guardiola, J. N., A. Zuker:
The spectra of mixed ^{3}He-^{4}He droplets, J. Chem. Phys. **123**, 054503 (2005)



Helium is the only substance that remains liquid down to T=0

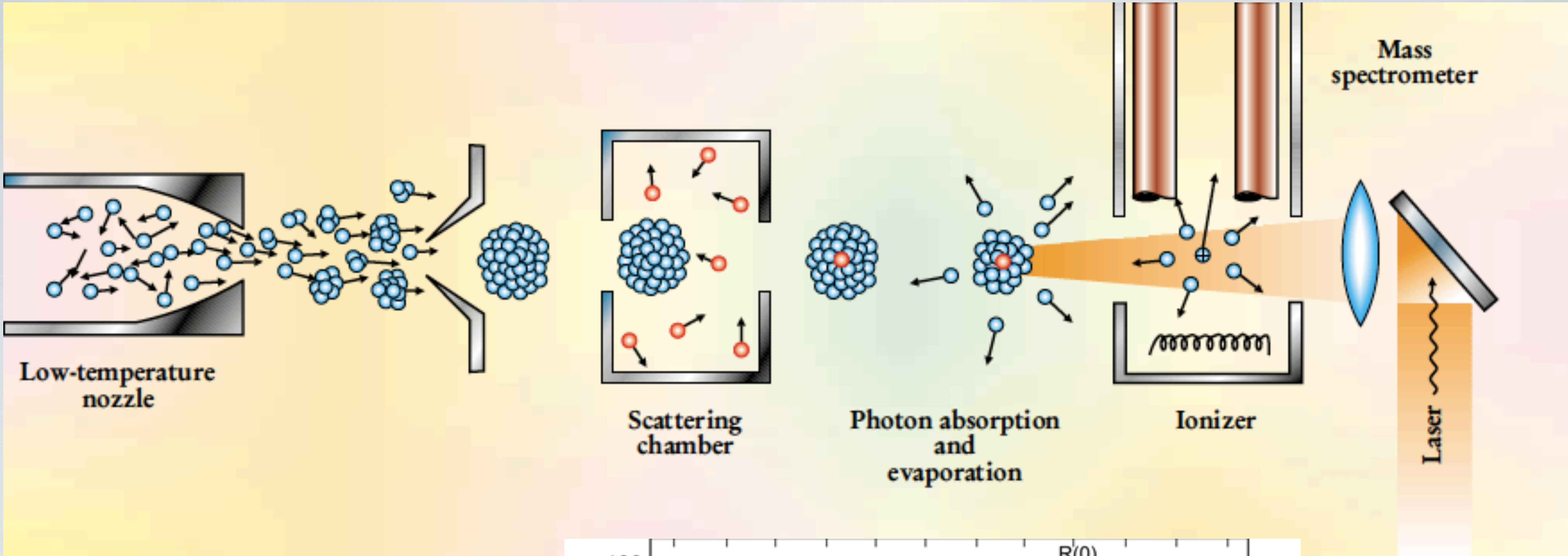
- Large zero-point motion
- Weak atom-atom attraction

Superfluid phase transition

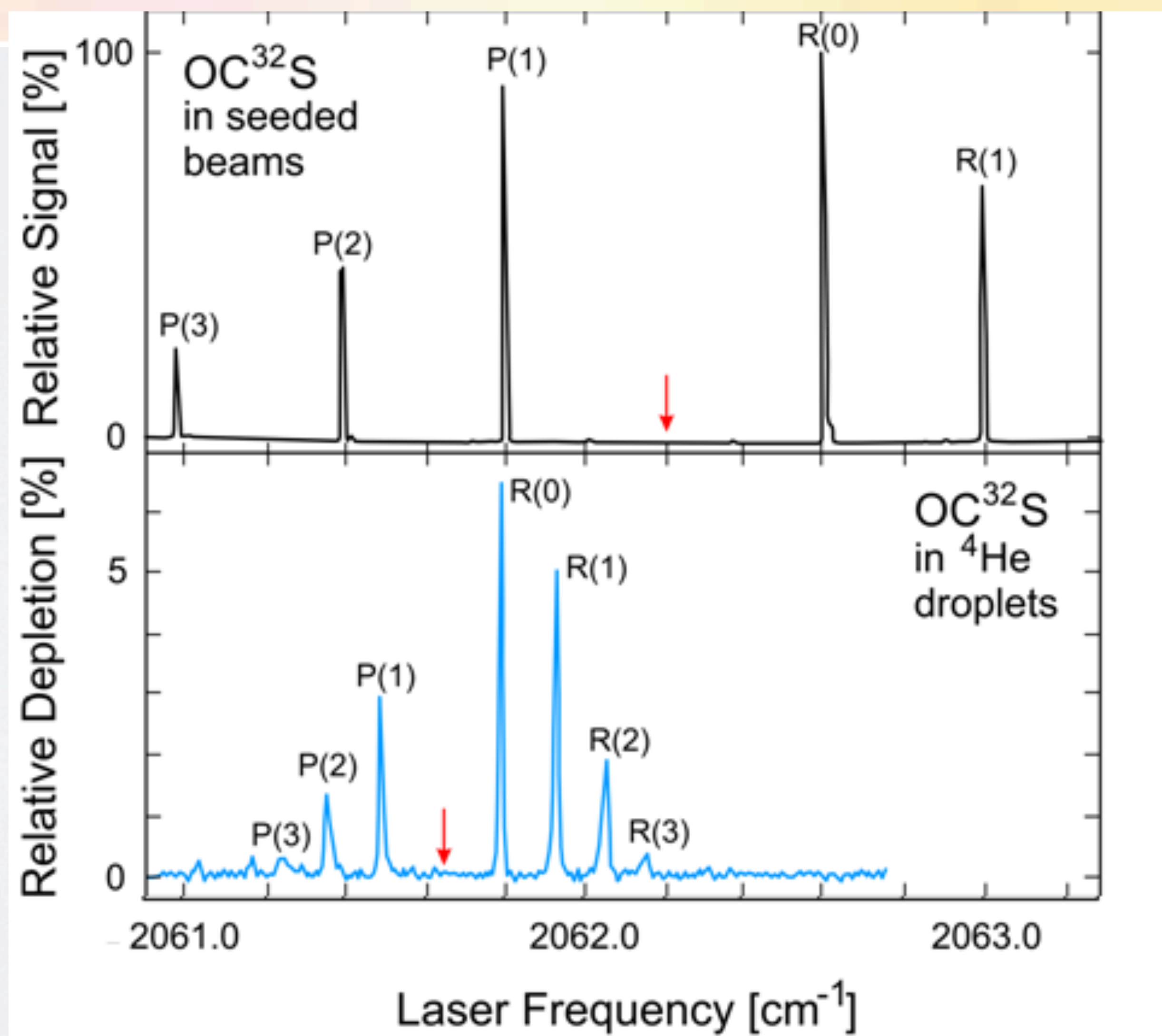
^{4}He T_λ = 2.2 K

^{3}He T_λ = 3 mK

1960's: is it possible to observe superfluidity in finite systems?



^{4}He droplets
T ≈ 0.36K
(superfluid)
^{3}He droplets
T ≈ 0.10K
(normal fluid)



OCS molecules rotate “freely” inside ^{4}He droplets

Size distribution in the jet: log-normal distribution
Typical average size: **a few thousand atoms**

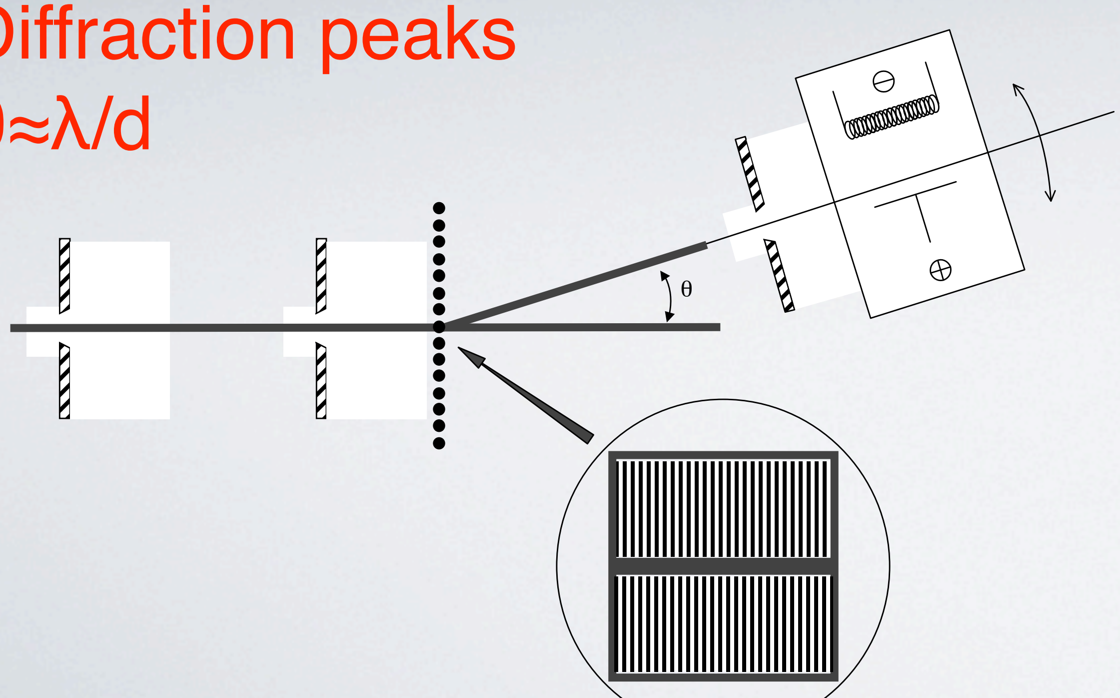
Detection of small droplets
(up to ≈ 40 amu)

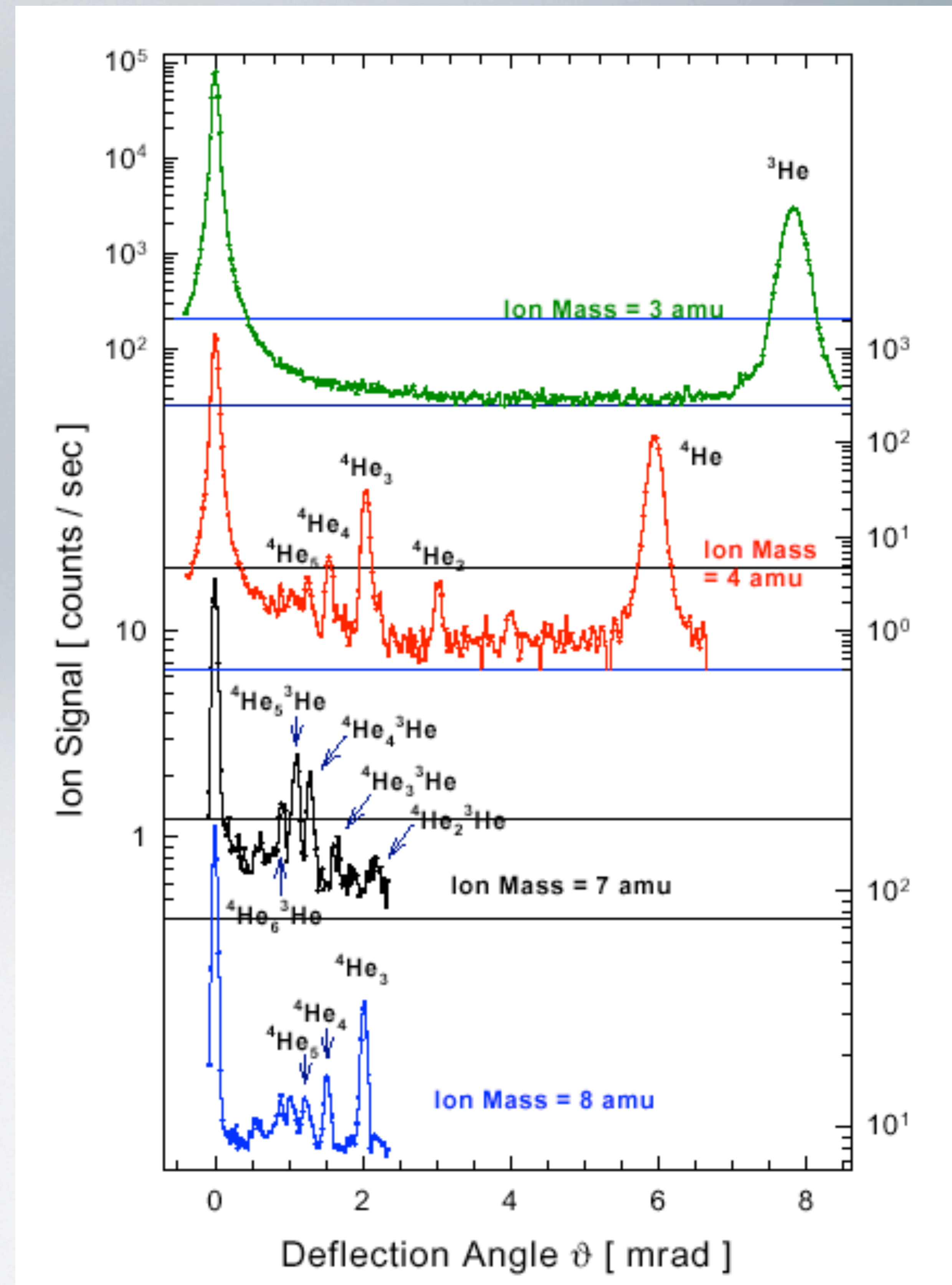
Atoms in the beam have
a sharp velocity $\Delta v/v \approx 2\%$

(W. Schöllkopf, J.P. Toennies, Science 266, 1345, 1994)

De Broglie wavelength
$\lambda = h/(Nmv)$
Typical value 0.1/N Å

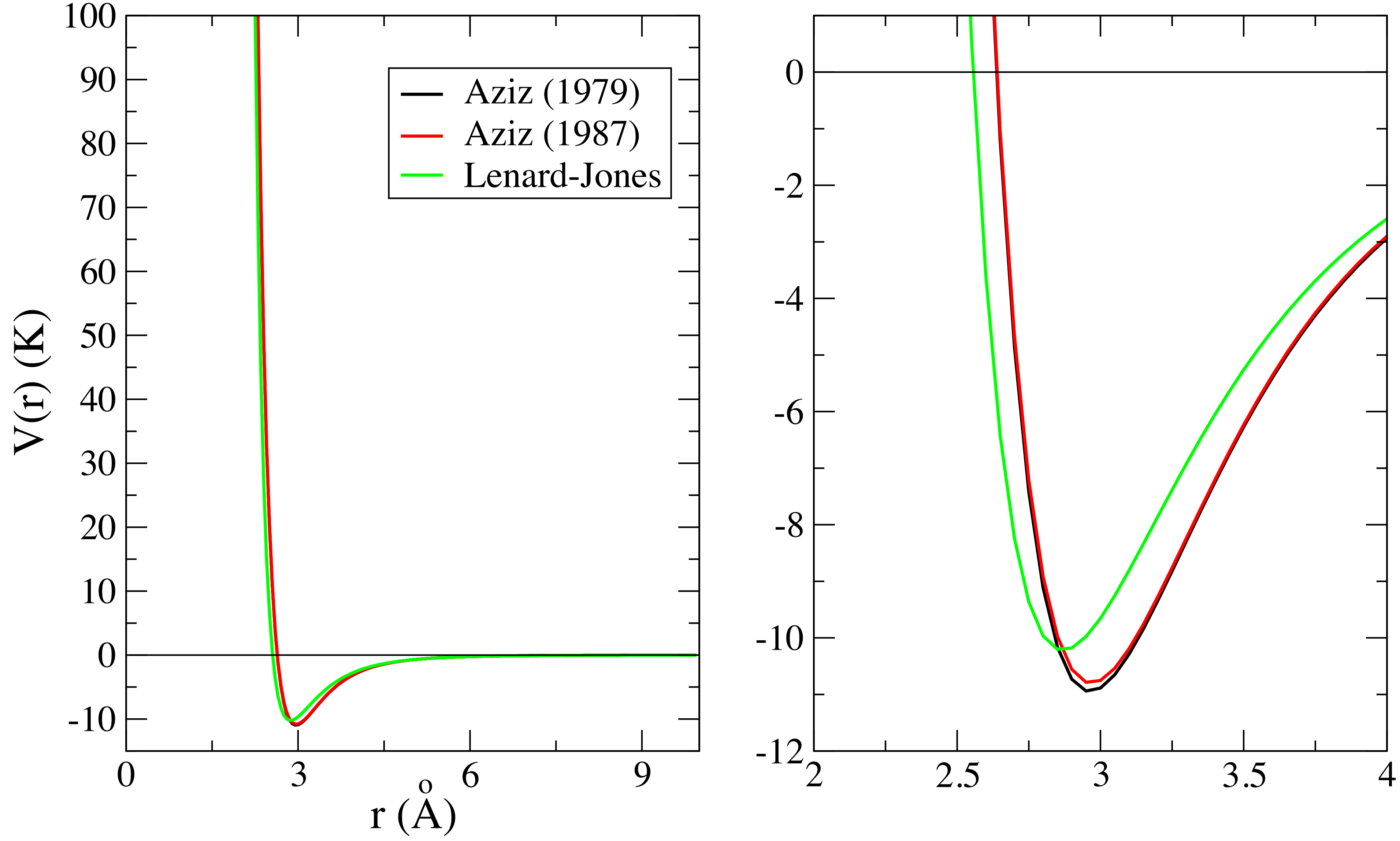
Diffraction peaks
$\theta \approx \lambda/d$





He-He interaction

1K ≈ 0.9 meV, 1Å $=10^5$ fm



Lowest excited state
≈ 20 eV ≈ 2.3 10^5 K

Structureless
- **bosons (^{4}He)**
- **fermions (^{3}He)**

Calculating dimers:

$^4He_2 \approx 1.3$ mK

$^3He_2$ unbound

^3He ^4He unbound

Diffraction experiment $^4He_2$

bond length

52 ± 4Å

binding energy

1.1+0.3-0.2 mK

Nuclear matter

E/N = -16 MeV

Deuteron

E/N = -1 MeV

^{4}He liquid

E/N = -7.5 K

$^4He_2$ dimer

E/N = -0.6 mK

^{3}He liquid

E/N= -2.5 K

$^3He_2$ dimer

unbound

↓

Minimum number of ^{3}He atoms to form a self-bound system

Theoretical methods to study Helium droplets

$^4He_{N4}$ // $^3He_{N3}$ // $^4He_{N4}$-$^3He_{N3}$

- Density functional theory

  Phenomenological interaction

$$E = \int dV\, \varepsilon(\rho_4, \rho_3)$$

- Monte Carlo simulations

  Microscopic He-He interaction

Shell model techniques

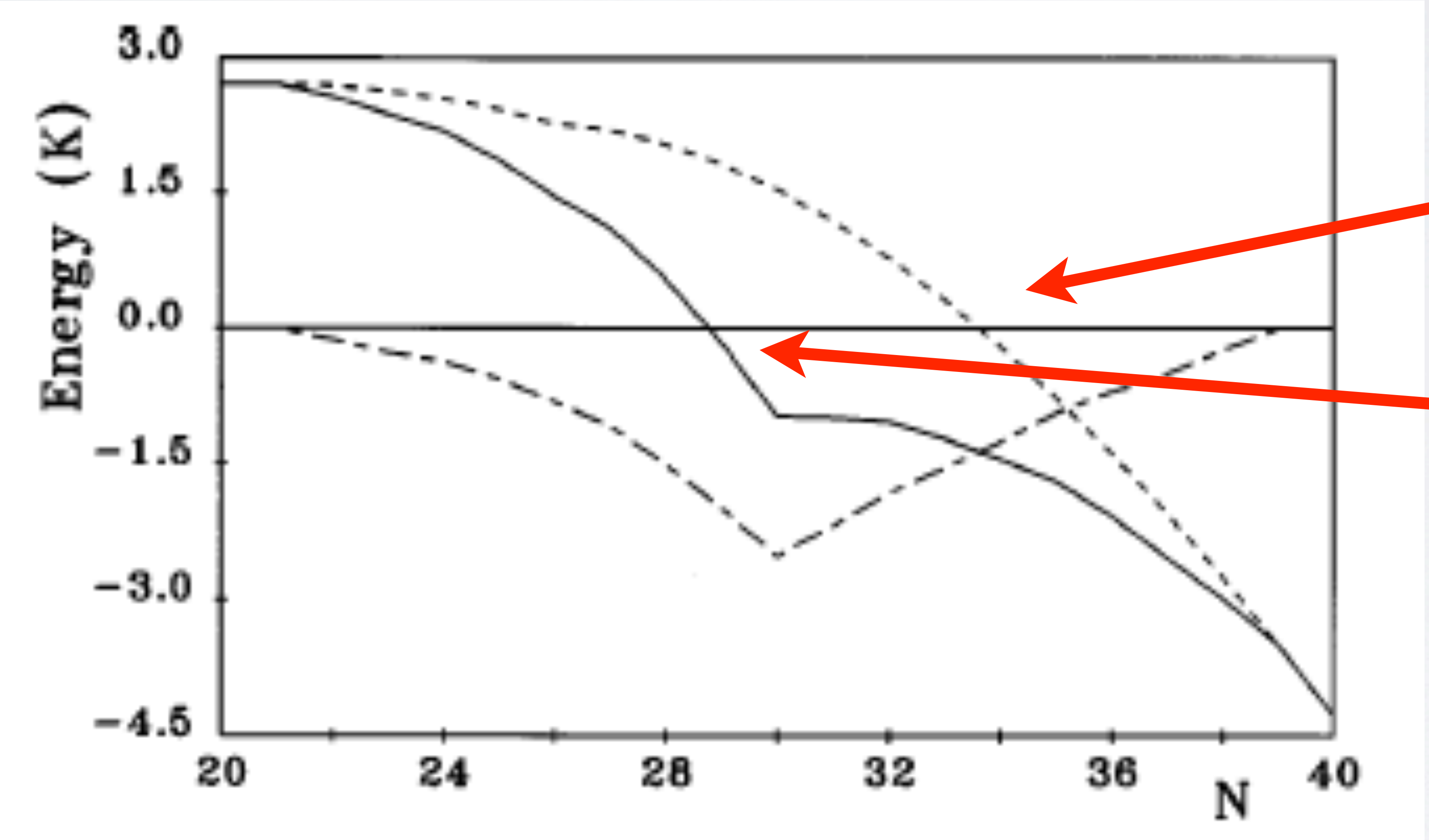
to describe certain properties

of fermionic (^3He) components

1. - Minimum number of ^{3}He atoms to form a bound droplet

Density functional
magic numbers: (p+1)(p+2)(p+3)/3

N_3=20 Unbound
N_3=40 Bound



Uniform filling approximation:
N_{min} = 34

Configuration interaction
(1f 2p shells)
DFT: ϕ_{nl}, ε_{nl}, V_{eff}
N_{min} = 29

However: Uncertainties in DF
+ Pronounced minimum in E_{corr}

Safe estimate: **N_{min} = 30**

TABLE II. Matrix elements $\langle l_1, l_2(L)|V|l_3, l_4(L)\rangle$ (K) for N = 30 and 40 drops.

l_1, l_2, l_3, l_4	LS	$N = 30$	$N = 40$
3, 3, 3, 3	00	0.724	0.896
	11	−0.247	−0.228
	20	−0.019	−0.010
	31	−0.210	−0.235
	40	0.015	0.024
	51	−0.203	−0.239
	60	0.010	−0.003
1, 1, 1, 1	00	0.307	0.506
	11	−0.137	−0.155
	20	−0.018	0.081
3, 1, 3, 1	20	−0.024	−0.012
	21	−0.237	−0.264
	30	−0.197	−0.245
	31	−0.188	−0.264
	40	−0.005	−0.053
	41	−0.235	−0.287

Diagonal M.E.

S=0, L=0
repulsive

S=1, L odd
attractive

S=0, L even >0
very small

$$\int d\mathbf{r}'\rho(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')$$

$$\text{Zero range}: V(\mathbf{r}) = t_0\delta(\mathbf{r})$$

Finite range :

$$V(\mathbf{r}) = 0\,, r < h$$

$$= V_{\mathrm{He-He}}(\mathbf{r})\,, r > h$$

Spin alignement due to short-range repulsion

Maximum spin in the open shell:
below mid-shell: $n_p/2$
above midshell: $n_h/2$

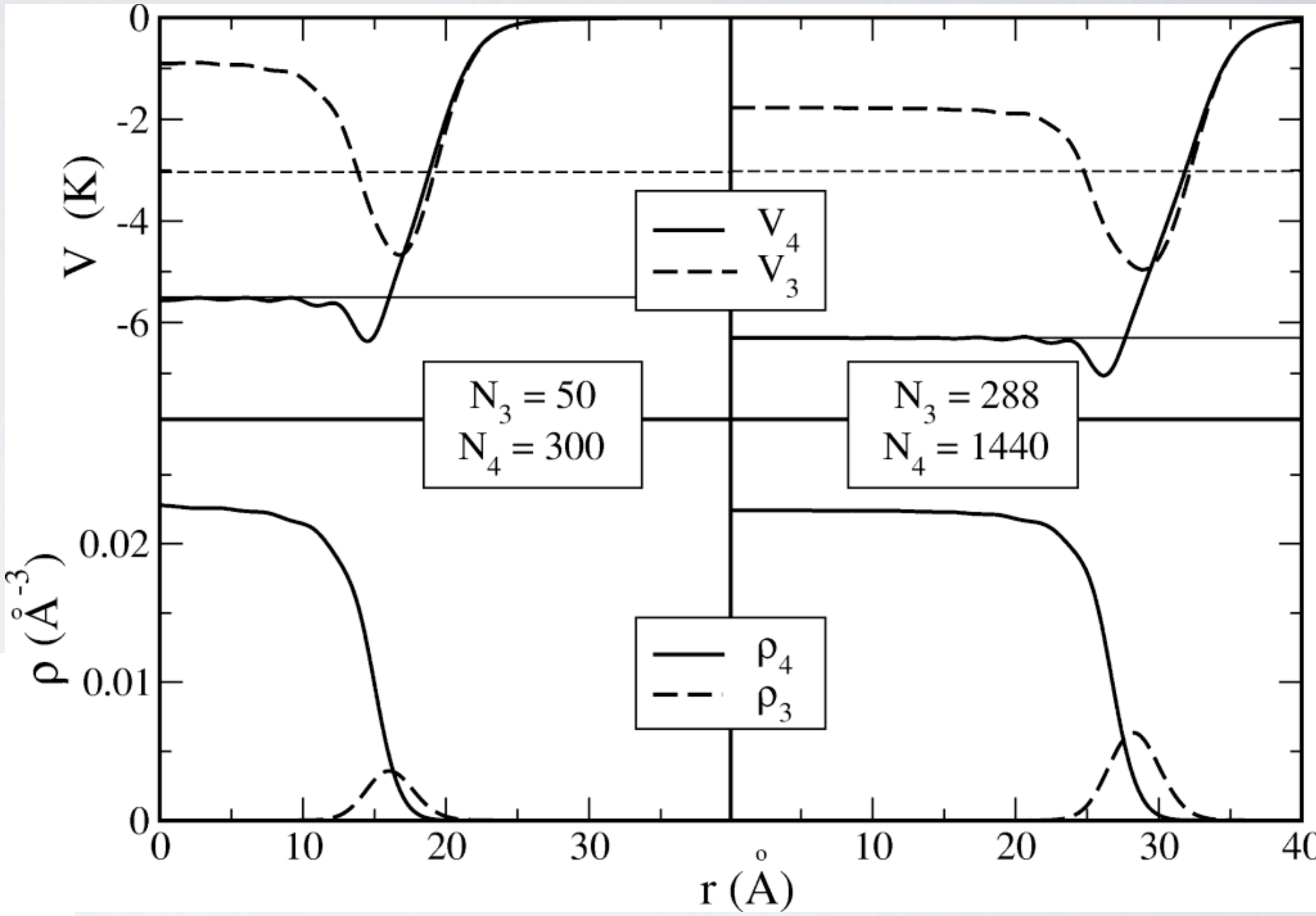
2. - Mixed ^{3}He-^{4}He droplets: density functional

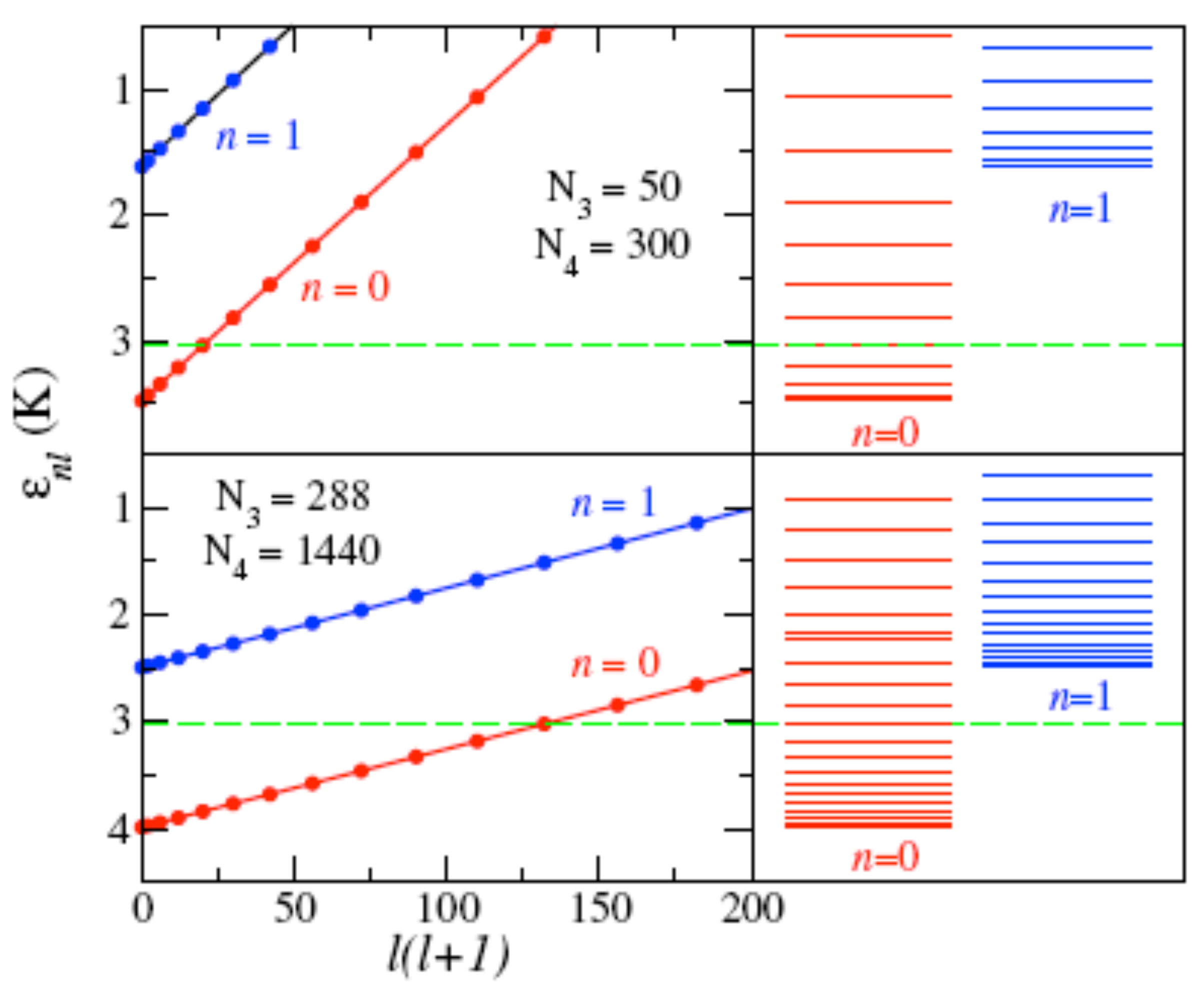
^{4}He atoms:
extra binding for ^{3}He atoms

$$\left[-\frac{\hbar^2}{2m_4}\frac{d^2}{dr^2}+V_4(r)\right]\sqrt{\rho_4(r)}=\mu_4\sqrt{\rho_4(r)}$$

$$\left[-\frac{\hbar^2}{2m_3^*}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)-\frac{d}{dr}\left(\frac{\hbar^2}{2m_3^*}\right)\frac{d}{dr}\right]\phi_{nl}(r)$$
$$+\left[V_3(r)+\frac{\hbar^2}{2m_3^*}\frac{l(l+1)}{r^2}\right]\phi_{nl}(r)=\epsilon_{nl}\phi_{nl}(r)$$

Perturbative term





Magic numbers
2 $(p+1)^2$, p=0, 1, ...
Levels:
$1s^2$, $1p^6$, $1d^{10}$, $1f^{14}$, ...

Configuration interaction (1g-1h shells)

TABLE I. Antisymmetrized two-body matrix elements $\langle l_i, l_j; L, S|V|l_m, l_n; LS\rangle$ in mK for the (50,300) droplet.

l_i	l_j	l_m	l_n	L	$S=0$	L	$S=1$
4	4	4	4	0	+83	1	−67
				2	+11	3	−26
				4	+6	5	−16
				6	+1	7	−10
				8	−11		
4	5	4	5	1	+111	1	−81
				2	−17	2	−80
				3	+30	3	−8
				4	−3	4	−47
				5	+15	5	−2
				6	−1	6	−32
				7	+5	7	−1
				8	0	8	−23
				9	−21	9	−2
5	5	5	5	0	+142	1	−93
				2	+18	3	−38
				4	+12	5	−24
				6	+7	7	−18
				8	+3	9	−13
				10	−11		

Analogous to the case of pure ^3He droplets

^3He atoms in the open shell couple to maximum spin

3. - Mixed ^{3}He-^{4}He droplets: diffusion Monte Carlo

Solve the Schrödinger equation in imaginary time

$$f(\mathcal{R},t) = \Psi_T(\mathcal{R})\Psi(\mathcal{R},t)$$

$$f(\mathcal{R},t+\Delta t) = \int d\mathcal{R}'\, G(\mathcal{R},\mathcal{R}',\Delta t)\, f(\mathcal{R}',t)$$

$$\Psi_T(\mathcal{R}) = \Psi_{BB}\Psi_{BF}\Psi_{FF}D_F \qquad \Psi_{MN} = \Pi_{i\neq j}\mathrm{e}^{f(r_{ij})}$$

Slater determinant $r^\ell Y_{\ell,m}$ Levels: $1s^2$, $1p^6$, $1d^{10}$, $1f^{14}$, ...

Consider levels: S_{max} , L_{max}

Other Technicalities:

Fixed-node approximation

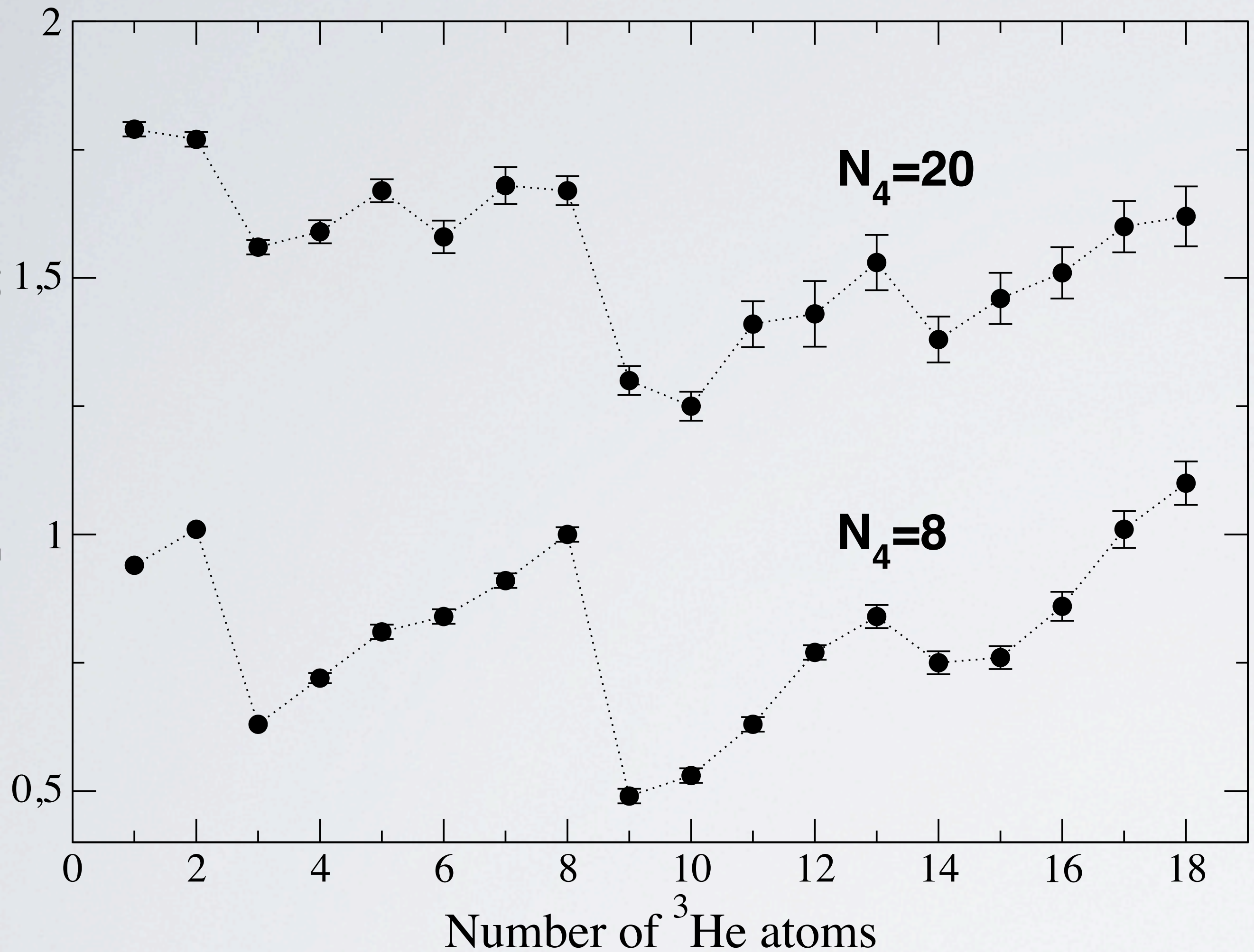
"Backflow" correlations $\mathbf{r}_i \rightarrow \mathbf{r}_i + \sum_{j\neq i} \eta(r_{ij})(\mathbf{r}_j - \mathbf{r}_i)$

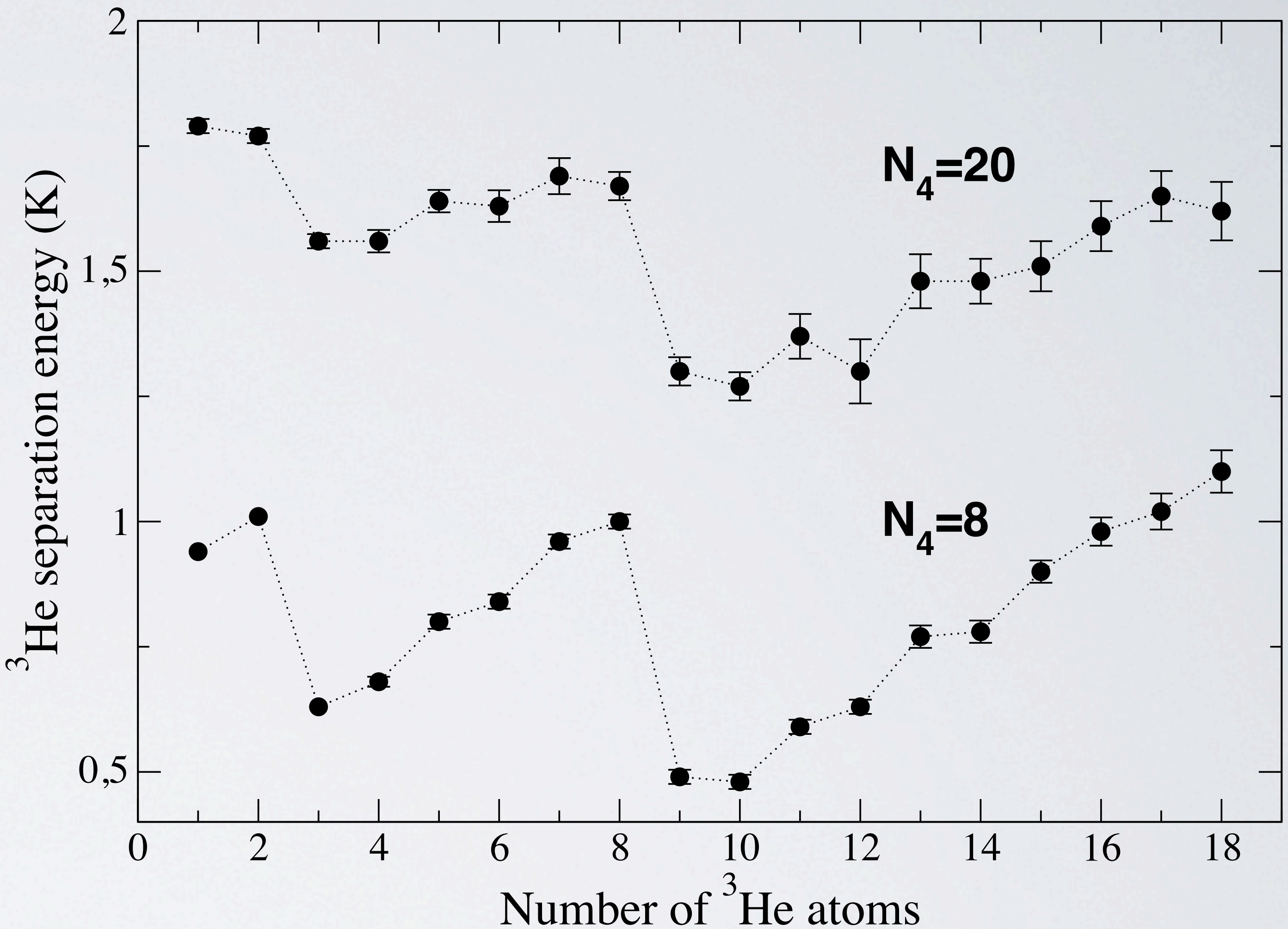
(to improve nodal surfaces)

DMC energies (in K)

N_F	Configuration	L	S	N_B=8	N_B=20
0		0	0	5.14(0)	33.76(1)
1	$1s^1$	0	1/2	6.08(0)	35.55(1)
2	$1s^2$	0	0	7.09(0)	37.32(1)
3	$1p^1$	1	1/2	7.72(0)	38.88(1)
4	$1p^2$	1	1	8.44(1)	40.47(2)
		2	0	8.40(1)	40.44(2)
5	$1p^3$	0	3/2	9.25(1)	42.14(1)
		2	1/2	9.20(1)	42.08(2)
6	$1p^4$	1	1	10.09(1)	43.72(3)
		2	0	10.04(1)	43.71(2)
7	$1p^5$	1	1/2	11.00(1)	45.40(2)
8	$1p^6$	0	0	12.00(1)	47.07(2)
9	$1d^1$	2	1/2	12.49(1)	48.37(2)
10	$1d^2$	3	1	13.02(1)	49.62(2)
		4	0	12.97(1)	49.64(4)
11	$1d^3$	3	3/2	13.65(1)	51.03(4)
		5	1/2	13.56(1)	51.01(3)
12	$1d^4$	2	2	14.42(1)	52.46(5)
		6	0	14.19(1)	52.23(4)
13	$1d^5$	0	5/2	15.26(2)	53.99(2)
		6	1/2	14.96(2)	53.71(3)
14	$1d^6$	2	2	16.01(1)	55.37(4)
		6	0	15.74(2)	55.19(4)
15	$1d^7$	3	3/2	16.77(2)	56.83(3)
		5	1/2	16.64(1)	56.70(5)
16	$1d^8$	3	1	17.63(2)	58.34(4)
		4	0	17.62(2)	58.29(4)
17	$1d^9$	2	1/2	18.64(3)	59.94(3)
18	$1d^{10}$	0	0	19.74(3)	61.56(5)

^{3}He separation energies
$E(N_B,N_F-1)-E(N_B,N_F)$





S_{max} L_{max}

An effective monopole Hamiltonian analysis

$$U = \sum_s n_s \varepsilon_s \qquad V^{LS}_{rs;tu} = \langle rs; LS|V|tu; LS\rangle$$

Hamiltonian: $H = H_{mS} + H_M$

H_{mS} gives the average energy of configurations at fixed number of particles and spin

$$V^S_{rs} = \frac{\sum_L V^{LS}_{rs;rs}(2L+1)[1+(-)^{L+S}\delta_{rs}]}{\sum_L (2L+1)[1+(-)^{L+S}\delta_{rs}]}$$

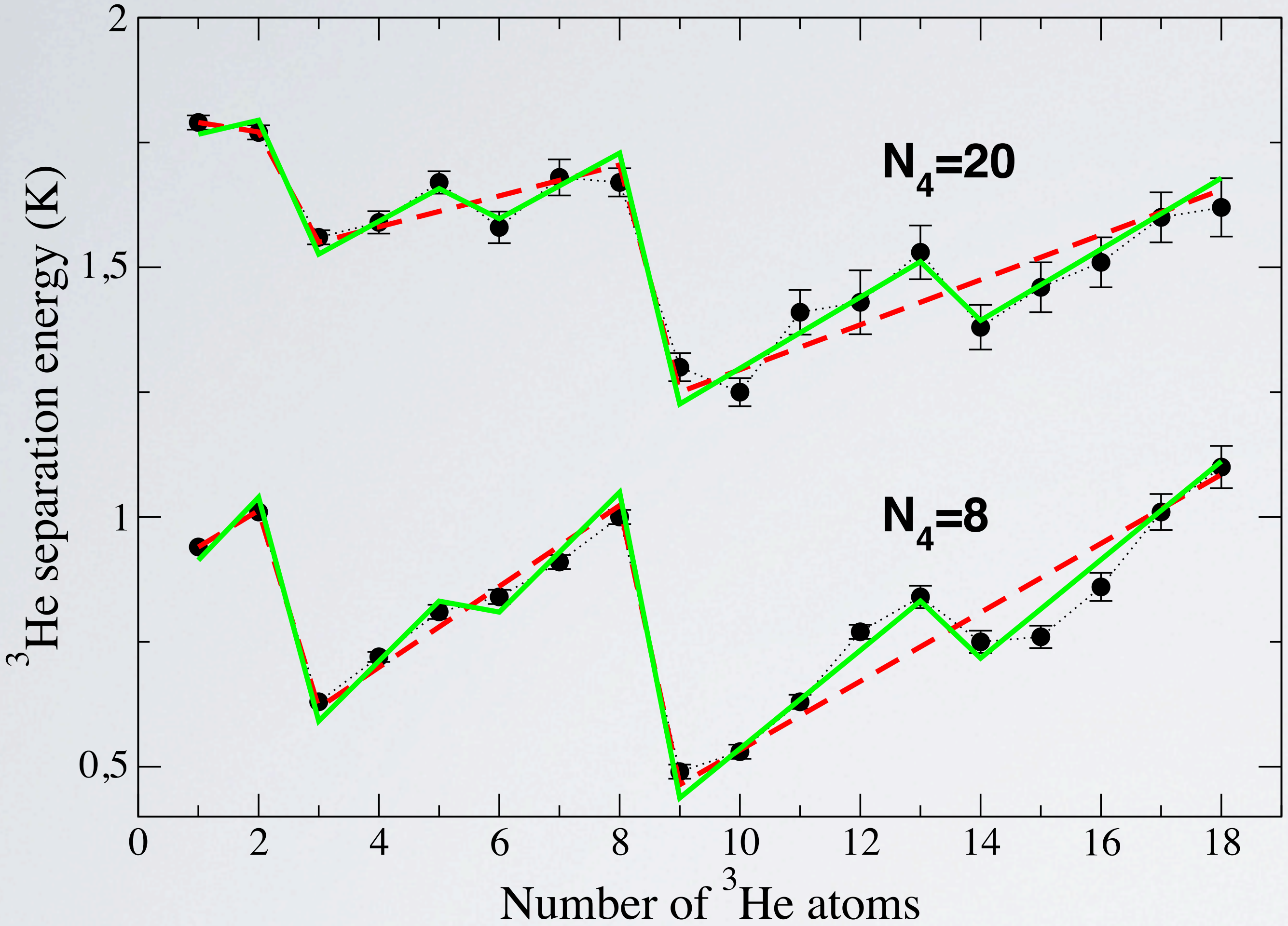
$$a_{rs} = \frac{1}{4}(3V^1_{rs} + V^0_{rs}) \, , b_{rs} = V^1_{rs} - V^0_{rs}$$

$$H_{mS} = U + \sum_{r \le s} \frac{1}{1+\delta_{rs}} \left[a_{rs} n_{rs}(n_{rs} - \delta_{rs}) + b_{rs} \left(\mathbf{S}_r \cdot \mathbf{S}_s - \frac{3n_r}{4}\delta_{rs} \right) \right]$$

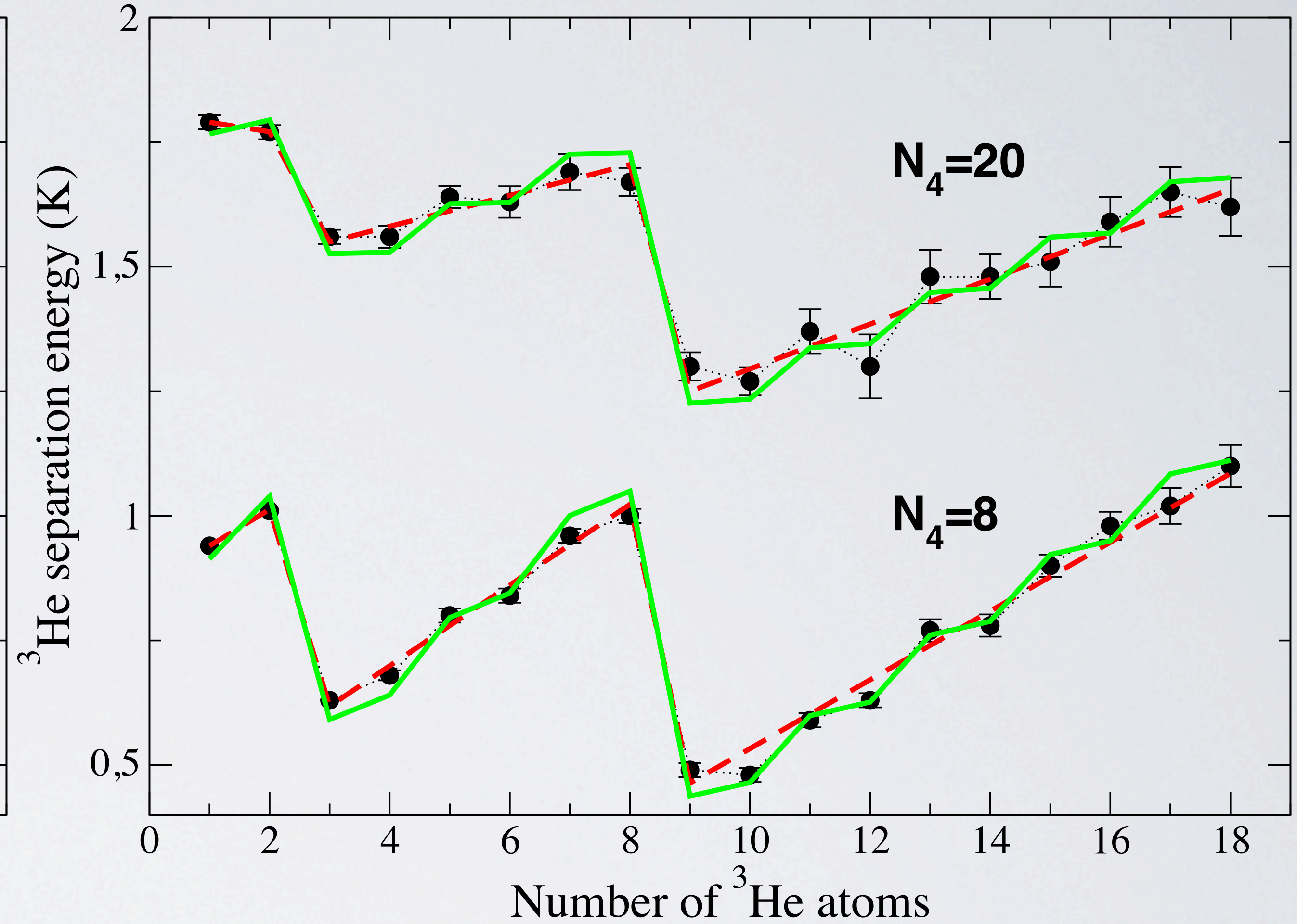
$$V_{rs} = a_{rs} - \frac{3}{4}\frac{\delta_{rs}}{D_r - 1} b_{rs} \, , D_r = 2(2\ell_r + 1) \qquad b_{rs} \to b$$

$$H_{mS} = U + \sum_{r<s} \frac{1}{1+\delta_{rs}} V_{rs} n_{rs}(n_{rs} - \delta_{rs}) + b \left[S(S+1) - \sum_r \frac{3n_r(D_r - n_r)}{4(D_r - 1)} \right]$$

S_{max}



L_{max}



V_{ss}, V_{pp}, V_{dd}, $(V_{sp}+3V_{sd})/4$, V_{pd}

Same + b

Simple interpretation of DMC energies in terms of H_{mS}

Helium droplets

- Interesting (interdisciplinary) many-body problem
- Structureless bosons and fermions, same interaction
- Effects related to different statistics and different masses

As compared with nuclei:
- Only central interaction
- Very correlated system (but a DFT works very well)

Shell model calculations:
- Stability threshold: 30 ^{3}He atoms
- ^{3}He atoms in the open shells coupled to maximum spin
- ^{3}He atoms in ^{3}He-^{4}He droplets: $1s^2$, $1p^6$, $1d^{10}$, $1f^{14}$, ...
- DMC results nicely interpreted in terms of monopolar Hamiltonian