# BEC: A "TAPAS" OF TOPICS

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# WHAT IS BOSE-EINSTEIN CONDENSATION ("BEC")?

What it is **NOT**: "$\langle\psi(\underset{\sim}{r})\rangle \neq 0$"

(never true for any system of conserved particles)

What it is (Penrose + Onsager 1956):

Consider single-particle density matrix

$$\rho(r,r':t) \equiv \int dr_2 \ldots dr_N\, \Psi^*(r_1 r_2 \ldots r_N : t)\, \Psi(r_1' r_2 \ldots r_N : t) \qquad (r_1 \equiv r,\ r_1' \equiv r')$$

$$\equiv \langle \psi^\dagger(r)\, \psi(r') \rangle (t)$$

Since $\rho$ Hermitian, can diagonalize:

$$\rho(r,r':t) = \sum_i n_i(t)\, \chi_i^*(r:t)\, \chi_i(r':t)$$

If all $n_i \sim O(1)$, no BEC $\qquad \equiv$ "0" $\qquad \equiv N_0$

If for one and **only** one $i$ $n_i \sim N$, "simple" BEC

If for more than one $i$ $n_i \sim N$, "fragmented" BEC.

For case of "simple" BEC **only**, define order parameter

$$\Psi(r:t) = \sqrt{N_0(t)}\, \chi_0(\underset{\sim}{r},t) \longleftarrow \equiv |\chi_0(rt)| \exp i\varphi(rt)$$

then

$$\underset{\sim}{v}_s(\underset{\sim}{r}t) \equiv \frac{\hbar}{m} \underset{\sim}{\nabla}\varphi(rt)$$

is "superfluid velocity"

$\rightarrow$ curl $\underset{\sim}{v}_s = 0$, $\oint v_s \cdot dl = nh/m$

Why should BEC ever happen?

[Contrast:

$v_n(r) \equiv \underset{\sim}{j}(\underset{\sim}{r}) / \rho(\underset{\sim}{r})$

$\neq \sum_i n_i \nabla\varphi_i(\underset{\sim}{r})$

$\Rightarrow$ curl $v_n(r) \neq 0$ ]

# Rigorous Theorems on BEC

(interacting system)

## 1. Existence at $T=0$

3D free space, pert$^n$ theory starting from noninteracting gas convergent: Gavoret + Nozières 1964

hard-core lattice gas at half filling: Kennedy et al. 1988.

## 2. Existence at $T \neq 0$

infinite-range interaction: Toth, Penrose 1992

no proof for short-range interactions
(?: Lieb + Seiringer Dec. 01)

## 3. Nonexistence at $T \neq 0$

free space, $d \leq 2$: Hohenberg 1967

many extensions to partially finite geometries, etc.

## 4. Upper bound on $f \equiv N_0/N$

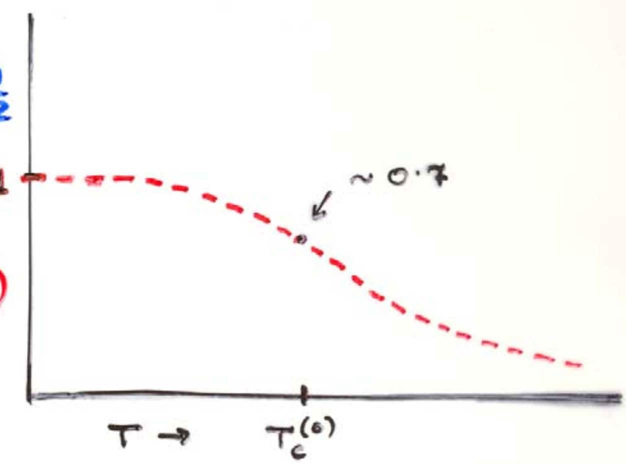
Hohenberg's lemma: (general for velocity-ind$^t$ interactions):

$$\langle n_k \rangle \geq \left(\frac{m k_B T}{\hbar^2 k^2}\right) f - \frac{1}{2}$$

3D free space: $\Rightarrow$

$$\frac{f}{(1-f)^{2/3}} \leq \gamma\left(T_c^{(0)}/T\right)$$

(Roepstorff (1978): $\gamma \approx 2$)



# (RIGOROUS) THEOREMS ON BEC, cont.

5. Part$^n$ theory (nonrigorous!) suggests repulsive interactions increase $T_c$ : specifically, (3D free space)

$$\Delta T_c / T_c^{(0)} = \text{const.}\ (n a_s^3)^{1/3}$$

(e.g. Baym et al. 2000).

**QUESTION:** Can we derive an upper bound on $f$ which is tighter than the Hohenberg-derived one, and in particular tends to the free-gas value for interaction $\Rightarrow 0$ ?

**ANSWER:** Yes, at least for a simple model of interactions. (A.J.L., New Journ. of Physics $\underset{=}{3}$, 23 (2001))

Model: $N$ spinless bosons in vol. $\Omega$, $N, \Omega \to \infty$,

$N/\Omega \to$ const. $\equiv n$.

Interaction: $\frac{1}{2}\sum_{ij} V(\underset{\sim}{r}_i - \underset{\sim}{r}_j)$, $V(\underset{\sim}{r}) \geq 0$, $\forall \underset{\sim}{r}$

Method:

Consider free energy $F(N)$ ($\equiv -k_B T \ln \mathrm{Tr}_N \exp - \hat{H}/kT$)

(i) Derive ($f$-independent) upper limit on $F$. ($F_{max}$)

(ii) Derive ($f$-dependent) lower limit on $F$. ($F_{min}(f)$)

(iii) Then $F_{min}(f) \leq F_{max} \Rightarrow$ upper bound on $f$.

(Assume, for simplicity only, that condensation is "simple" + occurs in $\underset{\sim}{k} = 0$ state)

## Step 1: Upper bound on $F(N)$

From "Hartree-Fock" variational ansatz,

$$\hat{\rho}_N = Z^{-1} \exp - \beta \hat{H}_0 \equiv \hat{\rho}_N^{(0)}$$

KE only

$$\Rightarrow \quad F(N) \leq F_0(N) + \tfrac{1}{2}\Big(N n V_0 + \Omega^{-1} \sum_{k \neq k'} V_{\underset{\sim}{k} - \underset{\sim}{k}'} \langle n_k \rangle \langle n_{k'} \rangle\Big)$$

"Hartree" "Fock"

since $V(r) \geq 0$, $V_k \leq V_0$, $\forall \underline{k}$ $\quad V_0 \equiv \int V(\underset{\sim}{r})\, d^3\underset{\sim}{r}$

$\Rightarrow$

$$F(N, \Omega, T) \leq F_0(N, \Omega, T) + N n V_0 \equiv F_{max}$$

## Step 2: Lower bound on $F(N)$

Principle: $F(N, \Omega, T)$ cannot be less than $F_0(N(1-f), \Omega, T)$, otherwise we could construct a density matrix $\hat{\rho}_{N(1-f)}^{(0,\,\text{trial})}$ which does better for the noninteracting gas with $N(1-f)$ particles than the standard one $\hat{\rho}_{N(1-f)}^{(0)}$ !

Proof: apply to true density matrix $\hat{\rho}_N$ operator $\hat{Y} \equiv (a_0)^{\hat{N}_0} (\hat{N}_0 !)^{-1/2}$, i.e. ...

## RIGOROUS THEOREMS ON BEC, cont.

To create trial density matrix for noninteracting gas of $N(1-f) \equiv N - N_0$ particles, start with exact density matrix of N particles and remove all the particles in the condensate, leaving rest unchanged*.

(Technically: $\hat{\rho}_{\text{trial}} \equiv \hat{Y} \hat{\rho}_N \hat{Y}^\dagger$ )

$$\left\{\begin{array}{l} \text{KE unchanged (since } \epsilon_0 \equiv 0) \\ \text{Entropy unchanged } (1 \to 1 \text{ mapping}) \\ \text{PE, originally } \geq 0 \text{, is identically zero for} \\ \qquad \text{noninteracting system} \end{array}\right.$$

$$\Rightarrow \quad F_0^{\text{trial}}(N(1-f), \Omega, T) \leq F(N, \Omega, T)$$

But, if $F_0^{\text{trial}} < F_0(N(1-f), \Omega, T)$, we have found a better density matrix for $N(1-f)$ particles than the "trivial" one $\hat{\rho}_{N(1-f)} \equiv Z^{-1} \exp - \beta \hat{H}_0$ !

Thus,

$$F(N, \Omega, T) \geq F_0(N(1-f), \Omega, T) \equiv F_{\min}(f)$$

* Technical complication: $[\hat{\rho}_N, \hat{N}_0] \neq 0$. See paper.

## Rigorous Theorems on BEC, cont.

We have proved:

(i) $F(N,\Omega,T) \leq F_0(N,\Omega,T) + NnV_0$

(ii) $F(N,\Omega,T) \geq F_0(N(1-f),\Omega,T)$

Thus,

$$\boxed{F_0(N(1-f),\Omega,T) - F_0(N,\Omega,T) \leq NnV_0}$$

free energy of noninteracting gas.

This is an implicit limit on $f$. To make it explicit, need to bound LHS below by an explicit function of $f$ (messy but straightforward).

Final result: $(T \geq T_c^{(0)})$

Limiting cases:

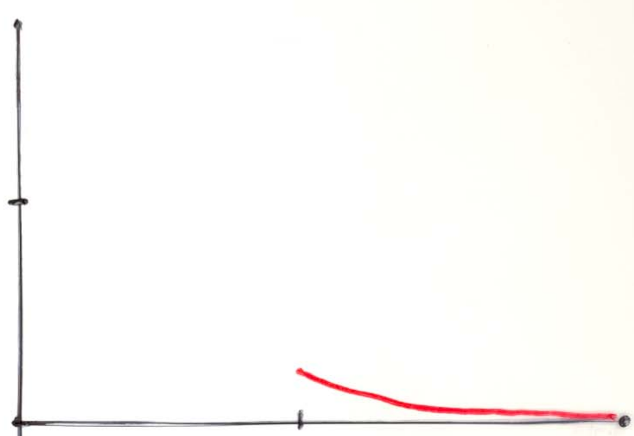
$T = T_c^{(0)}$: $f \leq \text{const.}\left(\frac{nV_0}{kT_c^{(0)}}\right)^{1/3}$

(const. $\cong 2.2$)

$\frac{nV_0}{kT_c^{(0)}} \ll 1 - T_c^{(0)}/T \ll 1$:

$$f \leq \text{const.}\,\frac{nV_0}{kT_c}\left(1-\left(\frac{T_c^{(0)}}{T}\right)^{3/2}\right)^{-2}$$

(const. $\cong 3.3$)



# Relation between GP and Bogoliubov Descriptions.

"Naive" approach:

2-particle interaction can be replaced by an effective pseudopotential

$$V_{eff}(r) = \frac{4\pi\hbar^2 a_s}{m}\delta(r) \equiv U_0\delta(r).$$

Then GP groundstate in free-space case is

$$\Psi_N = \frac{1}{\sqrt{N!}}(a_0^+)^N|vac\rangle$$

i.e. all particles condensed into plane-wave state $\underset{\sim}{k} = 0$.

Energy per particle is

$$(E/N)_{GP} = \tfrac{1}{2}nU_0 \qquad (*)$$

More general expression for energy is

$$E = \tfrac{1}{2}U_0\sum_{ij}|\Psi(r_i = r_j)|^2$$

So we would like to reduce $|\Psi(r_i=r_j)|^2$. To do this we allow scattering of particles out of condensate $(0,0 \to \underset{\sim}{k}, -\underset{\sim}{k})$, thereby obtaining the Bogoliubov groundstate with energy (in limit $na_s^3 \to 0$)

$$(E/N)_{Bog} = \tfrac{1}{2}nU_0(1 + A\cdot(na_s^3)^{1/2} + \ldots) \qquad (*)$$

↑ : $A > 0$ !! so if we take both results (*) seriously, GP is a better groundstate than Bogoliubov!

# RELATION BETWEEN GP AND BOGOLIUBOV DESCRIPTIONS (cont.)

Resolution of paradox (I think):

The general form of the Bogoliubov groundstate is

$$\Psi_N = \text{const.}\left(a_0^+ a_0^+ - \sum_k c_k a_k^+ a_{-k}^+\right)^{N/2}$$

which is (trivially) the <u>exact</u> form of the GS for N = 2.

The energy of the state $\Psi_N$ is

"Fock" term

$$(\dagger) \qquad E = \frac{1}{2}\frac{N^2}{V}U_0 + \sum_k \left\{ (\epsilon_k + nU_0)\frac{|c_k|^2}{1-|c_k|^2} - \frac{nU_0 c_k}{1-|c_k|^2} \right\}$$

For the 2-particle case, the "Fock" term is negligible and $c_k$ is of order $1/V$, so the solution is simply

$$c_k^{(2)} = \text{const.}\,(U_0/V)/\epsilon_k \sim V^{-1}k^{-2}$$

The "depletion" $\sum_{k\neq 0}|c_k|^2$ is $o(V^{-2}\sum_k k^{-4}) \sim V^{-1}k_{min}^{-1} \sim V^{-2/3}$ completely negligible.

Suppose now we take the GS in the GP approx$^n$ to be obtained by putting $c_k \to Nc_k^{(2)}$ (since $\langle N-2|a_0 a_0|N\rangle \sim N$) Then the depletion <u>diverges</u> as $N^2V^{-2}\sum_k k^{-4} \sim N^2V^{-2/3}$ $\sim N^{4/3}$, and the Fock term gives an energy per particle $\sim N^{1/3}$. I.e. if we define the GP state as above ($c_k \to Nc_k$) its energy is divergent! It is precisely to get rid of this divergence (<u>not</u> to lower the "Hartree" term) that we need to introduce the Bogoliubov ansatz (minimizing $(\dagger)$)

$$c_k = \frac{1}{nU_0}\left\{\epsilon_k + nU_0 - \sqrt{\epsilon_k(\epsilon_k + nU_0)}\right\}$$

Thus, the effect of the Bogoliubov corrections is to increase the probability of finding 2 atoms close together over the value it had in the 2-particle problem!

healing length

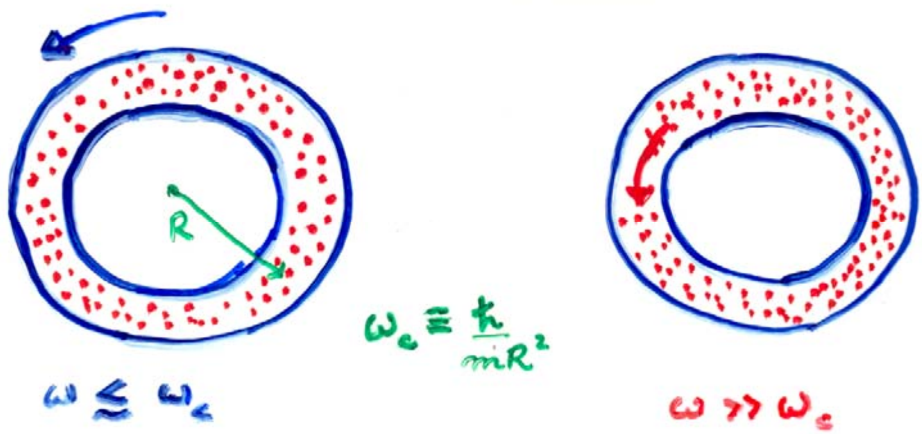
$$\psi_2(r) \sim 1 - \frac{a_s}{r} \qquad \psi_{Bg}(r) \sim 1 - \frac{a_s}{r} \exp - r/\xi$$

(cf: Yang + Lee 1956 (!)). Effect is to reduce the Fock term + thereby save overall energy.

Moral: $\exists$ no "GP approximation" in the sense of a well-defined ansatz for the MBWF!

# WHAT IS SUPERFLUIDITY? (contd.)

Rotational properties of $^4$He in annular geometry:




Hess-Fairbank effect:

rotate container ($\omega \lesssim \omega_c$), cool through $T_c$, liquid comes out of eq$^m$ with rotating container + to rest in lab. frame.

Must be **EQUILIBRIUM** effect.

Metastable supercurrents:

rotate container ($\omega \gg \omega_c$), cool through $T_c$. Liquid continues to rotate (almost) with container. Then stop container: liquid continues to rotate

Must be **METASTABLE** effect.

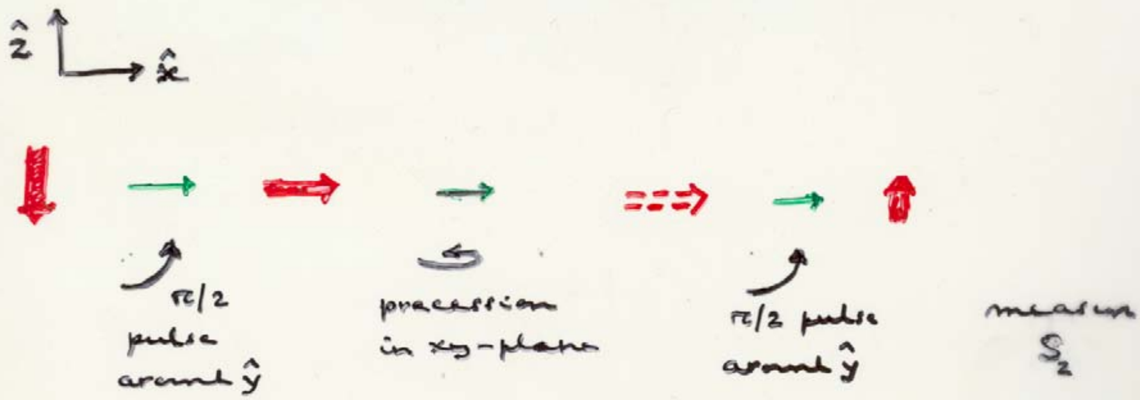
Fundamental principle: Equilibrium in container rotating with angular velocity $\underset{\sim}{\omega}$ obtained by minimizing

$$F(\underset{\sim}{\omega}) = \langle H_{eff} \rangle - TS,$$

$$\hat{H}_{eff} = \hat{H}_0 - \underset{\sim}{\omega} \cdot \underset{\sim}{\hat{L}}$$

# Detecting the Normal Component in Ramsey-Fringe Type Expts

JILA Ramsey-fringe expts: analogous to NMR.




Data given only for ensemble average of $S_z$, which decays in time. (attrib. phase diffusion).

Which is correct:

(a) System is at all times 100% Bose-condensed (as regards orbital degrees of freedom) but phase diffuses, or

(b) Condensate decreases with time?

How to tell? In real-life trap perhaps difficult, but consider ideal ("free-space") case, so no spatial inhomogeneity. Assume in absence of laser coupling $\hat{S}_z$ ($\equiv n_a - n_b$) conserved. Then:

(a) For 100% condensate, spin state must have $\hat{S}^2 = \frac{N}{2}\left(\frac{N}{2}+1\right)$, hence for $S_z = 0$,

$$|S_\perp| \sim N$$

bcos of chaotic behavior

but, of course, phase may be random from run to run.

(b) If all atoms normal, then exactly analogous to ordinary (liquid-state) NMR: $|\underset{\sim}{S}_\perp|$ should relax to zero with timescale $T_2$. So for $t \gg T_2$ expect measured value of $S_z$ at final stage to be <u>always</u> 0.

(c) If at given time $t$ fraction $f$ of atoms condensed, minimum value of $|S_\perp|$ is $2f-1$ (and "expected" value is $f$).

So, can we determine complete statistics of $|\underset{\sim}{S}_\perp|$?

(1) second $\pi/2$ pulse, this time around (appropriately "adjusted" in the light of first meas$^t$) $\hat{x}$-axis.
(First pulse measures $S_x$, second $S_y$: effectively commuting measurements for $N \gg 1$)

(2) statistics of existing meas$^{ts}$: are values of $S_z$ close to max. ($= N/2$) seen as often as expected?

Can one use existing measurements to set lower limit on combination of $\tau_{decoh}$ and $T_2$?

Real-life complication: $\Psi = \Psi(\underset{\sim}{r}, \underset{\sim}{\sigma} : t) \Rightarrow \underset{\sim}{S} = S(\underset{\sim}{r}, t)$

But, in BEC case, all atoms returning to same point at time $t$ have had the same (superposition of) histories $\Rightarrow S(r)$ still "large".

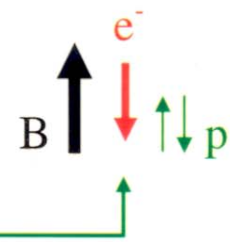
What is spatial extent of "coherence"?

# 4. THE SPIN-1/2 BOSE GAS: THE KSA* STATE

How can "Bose" atoms have spin ½?

Ex.: spin-polarized atomic H

$$\mu_B B \gg k_B T \gg \mu_n B$$




effectively fixed

Thought-expt. (Siggia & Ruckenstein, 1980):

Start at $T \gg T_c$, $\mu_n B \ll kT_c$. Then nuclei unpolarized,

$$\langle S_z^2 \rangle \sim \langle S^2 \rangle \sim N \quad (\underline{\text{not}} \sim N^2)$$

Now cool system through $T_c$, and down to $T = 0$, by collision processes which conserve spin.

What is the final state?

Paradox: If simple BEC, (i.e. all atoms condensed into single orbital state) then Bose statistics $\Rightarrow$ spin state of all atoms identical. But most general pure state of particle of spin ½ has $\underset{\sim}{\hat{n}} \cdot \underset{\sim}{\sigma} = \frac{1}{2}$ for some $\underset{\sim}{\hat{n}} \Rightarrow$ most general pure state of N bosons has

$$\underset{\sim}{S} = \frac{1}{2} N \underset{\sim}{n} \Rightarrow \langle S^2 \rangle \sim N^2$$

(mixtures don't help!)

*Kuklov-Svistunov-Ashhab

## SOLUTION (Kuklov-Svistunov, Ashhab, 2001):

With the given constraint,

"Simple" BEC is impossible!

In fact, the constrained groundstate is of the form

$$\Psi o \sim (a^{+}_{o\uparrow}\, a^{+}_{1\downarrow} - a^{+}_{o\downarrow}\, a^{+}_{1\uparrow})^{N/2}\, |vac\rangle$$

second lowest orbital state

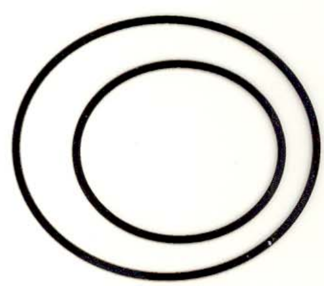
i.e.

Two orbital states are macroscopically occupied ("Fragmented BEC")

Spectacular example: (rough) annular geometry

i.e. no cons$^{n}$ of orbital ang. mom$^{m}$

Single-particle groundstate (s-state) is unique spinless Bose gas at rest. But first excited state in 2 degenerate states (p-states) related by TR.



So: What is "1" in above spin-1/2 GS?

Ans: in presence of weak repulsive interaction, 1 is either p or –p (not a combination) ⇒

SPONTANEOUS MACROSCOPIC ROTATION!

# BEC ALKALI GAS: "RAMSEY-FRINGE" EXPT. (SCHEMATIC)



2 different hyperfine species ~($\uparrow,\downarrow$): can be distinguished by absorption spectroscopy, so can measure "$\langle S_z \rangle$". Hyperfine splitting ~ $\mathcal{H}$ (magn. field).

Start with all atoms in the $\downarrow$ state:

$\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow$ $\quad\quad \Downarrow$

Apply $\pi/2$ RF pulse resonant with $\mathcal{H}$:

$$\downarrow \;\nearrow\; \rightarrow \quad \langle|\downarrow\rangle \longrightarrow \frac{1}{\sqrt{2}}\left(|\downarrow\rangle + |\downarrow\rangle\right)$$

$\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow$ $\quad\quad \Rightarrow$

wait for time t, then reverse $\pi/2$ pulse

(NMR analog: free-precession expt.)

What do we expect for $\langle S_z \rangle$ after 2nd pulse?

View from above:

A. Normal (uncondensed) system:

$\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow \;\rightarrow\; \searrow\searrow\searrow\searrow\searrow\searrow \;\rightarrow\; \swarrow\searrow\nwarrow\swarrow\nearrow\searrow$

$\Rightarrow$ PRECESSION $\searrow$ randomiz$^n$ over ~ $T_2$ $\Rightarrow$

So for $t \gtrsim T_2$ expect $\quad \downarrow \; \pi/2 \quad \Downarrow$

$\langle S_z \rangle \ll N$

## BOSE-CONDENSED SYSTEM:

Each atom must have some definite direction of spin in the xy-plane, and this direction must be the same for all N atoms!

$\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow$

$\boldsymbol{\rightarrow}$

"randomization" common to all N spins! $\rightarrow$

$\nearrow\nearrow\nearrow\nearrow\nearrow\nearrow$

$\boldsymbol{\nearrow}$

OR…

$\searrow\searrow\searrow\searrow\searrow\searrow$

$\boldsymbol{\searrow}$

OR…

$(\Psi \sim a_{\nearrow} |\nearrow\nearrow\nearrow \dots\rangle + a_{\searrow} |\searrow\searrow\searrow \dots\rangle + \dots)$

So: magnitude of total spin in xy-plane always N, direction indeterminate!

On second pulse at t,

$\boldsymbol{\rightarrow} \;\rightarrow\; \boldsymbol{\downarrow}, \quad \boldsymbol{\leftarrow} \;\rightarrow\; \boldsymbol{\uparrow}$, etc

So even for $t \gg T_2$,

$\langle S_z \rangle \sim N$ (But random from shot to shot)