Spin-3 Chromium Bose-Einstein Condensates

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We analyze the physics of spin-3 Bose-Einstein condensates, and in particular the new physics expected in on-going experiments with condensates of Chromium atoms. We first discuss the ground-state properties, which, depending on still unknown Chromium parameters, and for low magnetic fields can present various types of phases. We also discuss the spinor-dynamics in Chromium spinor condensates, which present significant qualitative differences when compared to other spinor condensates. In particular, dipole-induced spin relaxation may lead for low magnetic fields to transfer of spin into angular momentum similar to the well-known Einstein-de Haas effect. Additionally, a rapid large transference of population between distant magnetic states becomes also possible.

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Within the very active field of ultra cold atomic gases, multicomponent (spinor) Bose-Einstein condensates (BECs) have recently attracted a rapidly growing attention. Numerous works have addressed the rich variety of phenomena revealed by spinor BEC, in particular in what concerns ground-state and spin dynamics. The first experiments on spinor BEC were performed at JILA using mixtures of \(^{87}\)Rb BEC in two magnetically confined internal states (spin-1/2 BEC)\(^{10}\). Optical trapping of spinor condensates was first realized in spin-1 Sodium BEC at MIT\(^{11}\) constituting a major breakthrough since, whereas magnetic trapping confines the BEC to weak-seeking magnetic states, an optical trap enables confinement of all magnetic substates. In addition, the atoms in a magnetic substrate can be converted into atoms in other substates through interatomic interactions. Hence, these experiments paved the way towards the above mentioned fascinating phenomenology originating from the spin degree of freedom. Various experiments have been realized since then in spin-1 BEC, in particular in \(^{87}\)Rb in the \(F = 1\) manifold. It has been predicted that spin-1 BEC can present just two different ground states phases, either ferromagnetic or polar\(^{1}\). In the case of \(F = 1\) \(^{87}\)Rb it has been shown that the ground-state presents a ferromagnetic behavior\(^{13,14,15}\). These analyses have been recently extended to spin-2 BEC, which presents an even richer variety of possible ground-states, including in addition the so-called cyclic phases\(^{2,6}\). Recent experiments have shown a behavior compatible with a polar ground-state, although in the very vicinity of the cyclic phase\(^{13,19}\). Recently, spin dynamics has attracted a major interest, revealing the fascinating physics of the coherent oscillations between the different components of the manifold\(^{12,13,14,15,16,17}\).

Very recently, a Chromium BEC (Cr-BEC) has been achieved at Stuttgart University\(^{20}\). Cr-BEC presents fascinating new features when compared to other experiments in BEC. On one hand, since the ground state of \(^{52}\)Cr is \(^{7}\)S\(_{1}\), Cr-BEC constitutes the first accessible example of a spin-3 BEC. We show below that this fact may have very important consequences for both the ground-state and the dynamics of spinor Cr-BEC. On the other hand, when aligned into the state with magnetic quantum number \(m = \pm 3\), \(^{52}\)Cr presents a magnetic moment \(\mu = 6\mu_B\), where \(\mu_B\) is the Bohr magneton. This dipolar moment should be compared to alkali atoms, which have a maximum magnetic moment of \(1\mu_B\), and hence 36 times smaller dipole-dipole interactions. Ultra cold dipolar gases have attracted a rapidly growing attention, in particular in what concerns its stability and excitations\(^{21}\). The interplay of the dipole-dipole interaction and spinor-BEC physics has been also considered\(^{7,8}\). Recently, the dipolar effects have been observed for the first time in the expansion of a Cr-BEC\(^{22}\).

This Letter analyzes spin-3 BEC, and in particular the new physics expected in on-going experiments in Cr-BEC. After deriving the equations that describe this system, we focus on the ground-state, using single-mode approximation (SMA), showing that various phases are possible, depending on the applied magnetic field, and the (still unknown) value of the \(s\)-wave scattering length for the channel of total spin zero. This phase diagram presents certain differences with respect to the diagram first worked out recently by Diener and Ho\(^{22}\). In the second part of this Letter, we discuss the spinor dynamics, departing from the SMA. The double nature of Cr-BEC as a spin-3 BEC and a dipolar BEC is shown to lead to significant qualitative differences when compared to other spinor BECs. The larger spin can allow for fast population transfer from \(m = 0\) to \(m = \pm 3\) without a sequential dynamics as in \(F = 2\) \(^{87}\)Rb\(^{18}\). In addition, dipolar relaxation violates spin conservation, leading to...
rotation of the different components, resembling the well-known Einstein-de Haas (EH) effect [2].

In the following we consider an optically trapped Cr-BEC with N particles. The Hamiltonian regulating Cr-BEC is of the form $\hat{H} = \hat{H}_0 + \hat{V}_{sr} + \hat{V}_{dd}$. The single-particle part of the Hamiltonian, $\hat{H}_0$, includes the trapping energy and the linear Zeeman effect (quadratic Zeeman effect is absent in Cr-BEC), being of the form

$$\hat{H}_0 = \int d\mathbf{r} \sum_m \hat{\psi}_m^\dagger(\mathbf{r}) \left[ \frac{-\hbar^2}{2M} \nabla^2 + U_{trapping}(\mathbf{r}) + pm \right] \hat{\psi}_m(\mathbf{r}),$$

(1)

where $\hat{\psi}_m^\dagger$ ($\hat{\psi}_m$) is the creation (annihilation) operator in the $m$-state, $M$ is the atomic mass, and $p = g_\mu_B B$, with $g = 2$ for $^{52}$Cr, and $B$ is the applied magnetic field.

The short-range (van der Waals) interactions are given by $\hat{V}_{sr}$. For any interacting pair with spins $S_{1,2}$, $\hat{V}_{sr}$ conserves the total spin, $S$, and is thus described in terms of the projector operators on different total spins $\hat{P}_S$, where $S = 0, 2, 4$, and 6 (only even $S$ is allowed) [11]:

$$\hat{V}_{sr} = \frac{1}{2} \int d\mathbf{r} \sum_{S=0}^6 g_S \hat{P}_S(\mathbf{r}),$$

(2)

where $g_S = 4\pi\hbar^2 a_S/M$, and $a_S$ is the $S$-wave scattering length for a total spin $S$. Since $S_1 \cdot S_2 = (S^2 - S_1^2 - S_2^2)/2$, then $\sum S \hat{P}_S(\mathbf{r}) = \hat{n}(\mathbf{r}) \hat{S}^2(\mathbf{r}) \hat{n}(\mathbf{r})$, and $\sum S \lambda_S^2 \hat{P}_S(\mathbf{r}) = \hat{O}^2(\mathbf{r}) \hat{n}(\mathbf{r})$, where $\hat{n}$ denotes normal order, $\lambda_S = [S(S + 1) - 24]/2 \hat{n}(\mathbf{r}) = \sum S \lambda_S^2 \hat{P}_S(\mathbf{r}) = \hat{O}^2(\mathbf{r}) \hat{n}(\mathbf{r})$, where $\hat{O} = \sum_{i=x,y,z} \hat{O}_i$.

For the case of $^{52}$Cr [22], $a_{0.2} = 112a_B$, where $a_B$ is the Bohr radius, and $c_0 = 0.65g_0$, $c_1 = 0.059g_0$, $c_2 = g_0 + 0.37g_0$, and $c_3 = -0.002g_0$. The value of $a_0$ is unknown, and hence, in the following, we consider different scenarios depending on the value of $g_0/g_6$. Note that Eq. (3) is similar to that obtained for spin-2 BEC [3, 4], the main new feature being the $c_3$ term, which introduce qualitatively new physics as discussed below.

The dipole-dipole interaction $\hat{V}_{dd}$ is of the form

$$\hat{V}_{dd} = \frac{c_d}{2} \int d\mathbf{r} \int d\mathbf{r}' \left[ \frac{1}{|\mathbf{r} - \mathbf{r}'|} \hat{\psi}_m^\dagger(\mathbf{r}) \hat{\psi}_m(\mathbf{r}') \hat{\psi}_{m'}^\dagger(\mathbf{r}') \hat{\psi}_{m'}(\mathbf{r}) \right] [S_{mn} \cdot S_{m'n'} - 3(S_{mn} \cdot \mathbf{e})(S_{m'n'} \cdot \mathbf{e})] \hat{n}(\mathbf{r}) \hat{n}(\mathbf{r}')$$

(4)

where $c_d = \mu_0 g_0^2 g_6^2/4\pi$, with $\mu_0$ the magnetic permeability of vacuum, and $\mathbf{e} = (\mathbf{r} - \mathbf{r}')/|\mathbf{r} - \mathbf{r}'|$. For $^{52}$Cr

$$c_d = 0.004g_6. \hat{V}_{dd} \text{ may be re-written as:}$$

$$\hat{V}_{dd} = \frac{\sqrt{3\pi}}{10} c_d \int d\mathbf{r} d\mathbf{r}' \left[ \hat{F}_{zz}(\mathbf{r}, \mathbf{r}') \hat{Y}_{20} + \hat{F}_{z\pm}(\mathbf{r}, \mathbf{r}') \hat{Y}_{21} + \hat{F}_{-z\pm}(\mathbf{r}, \mathbf{r}') \hat{Y}_{2-1} \right],$$

(5)

where $\hat{F}_{zz}(\mathbf{r}, \mathbf{r}') = \sqrt{2/3} [3\hat{F}_{z}(\mathbf{r}) \hat{F}_{z}(\mathbf{r}') - \hat{F}(\mathbf{r}) \cdot \hat{F}(\mathbf{r}')$, $\hat{F}_{z\pm}(\mathbf{r}, \mathbf{r}') = \pm[\hat{F}_{z}(\mathbf{r}) \hat{F}_{z}(\mathbf{r}') + \hat{F}_{z}(\mathbf{r}) \hat{F}_{z}(\mathbf{r}')]$, $\hat{F}_{-z\pm}(\mathbf{r}, \mathbf{r}') = \hat{F}_{z}(\mathbf{r}) \hat{F}_{z}(\mathbf{r}')$, $\hat{F}_{z} = \hat{F}_{z} \pm i\hat{F}_{y}$, and $Y_{2\mp}(\mathbf{r}, \mathbf{r}')$ are the spherical harmonics. Note that contrary to the short-range interactions, $\hat{V}_{dd}$ does not conserve the total spin, and may induce a transference of angular momentum into the center of mass (CM) degrees of freedom.

We first discuss the ground-state of the spin-3 BEC for different values of $g_0$, and the magnetic field, $p$. We consider mean-field (MF) approximation $\hat{\psi}_m(\mathbf{r}) \approx \sqrt{N} \hat{n}(\mathbf{r})$. In order to simplify the analysis of the possible ground-state solutions we perform SMA: $\hat{\psi}_m(\mathbf{r}) = \Phi(\mathbf{r}) \hat{n}(\mathbf{r})$, with $\int d\mathbf{r} |\Phi(\mathbf{r})|^2 = 1$. Apart from spin-independent terms the energy per particle is of the form:

$$E = pf_z + \frac{Nc_1\beta}{2} (f_z^2 + f_zf_-) + \frac{Nc_3\beta}{2} \left[ \frac{\sqrt{2/3}}{10} \Gamma_0 f_z^2 - f_zf_- \right]$$

$$+ \frac{Nc_3\beta}{2} \sum_{ij} \frac{\sqrt{3\pi}}{10} N \left[ \hat{n}(\mathbf{r}) \psi_m(\mathbf{r}_z) \psi_m(\mathbf{r}_z) \right],$$

(6)

where $\beta = \int d\mathbf{r} |\Phi(\mathbf{r})|^4$, $s_z = \frac{1}{2} \sum \hat{n}(\mathbf{r}) \psi_m(\mathbf{r}) \psi_{-m}(\mathbf{r})$, $f_z = \sum \hat{n}(\mathbf{r}) \psi_m^*(\mathbf{r}) \psi_{-m}(\mathbf{r})$, $O_{ij} = \sum \hat{n}(\mathbf{r}) \psi_m^*(\mathbf{r}) \psi_{m'}(\mathbf{r}) \psi_n(\mathbf{r})$, and $\Gamma_m = \int d\mathbf{r} d\mathbf{r'} |\Phi(\mathbf{r})|^2 |\Phi(\mathbf{r}')|^2 \hat{Y}_{2m}(\mathbf{r}) \hat{Y}_{2m}(\mathbf{r}')$. Note that $\Gamma_{\pm} = 0$ for any symmetric density $|\Phi(\mathbf{r})|^2$.

Let us consider a magnetic field in the $z$-direction. Hence, the ground-state magnetization must be aligned with the external field, and $f_+ = f_- = 0$. Then, we obtain that $\sum O_{ij}^2 = 77 - 12\gamma_z + 3\gamma_z^2/2 - f_z^2/2 + |\gamma|^2/2 + 2|\gamma|^2$, where $\gamma_z = \sum \hat{n}(\mathbf{r}) \psi_m(\mathbf{r})^2$, $\eta = \sum \hat{n}(\mathbf{r}) \psi_m(\mathbf{r})^2$, $\hat{\psi}_{m+2}$.

FIG. 1: Phase diagram function of $g_0/g_6$ and $\tilde{g}_6$, where $\tilde{g}_6 = 2g_\mu_B B/N\beta$. 

$S_{2;3,2} \text{ or } S_{3;3,1,1}$

$S_{2;3,1,1}$

$S_{3;3,1,1}$

$S_{2;3,1,1}$ or $S_{1;3,1,1}$

$S_{3;3,1,1}$

$S_{2;3,1,1}$

$S_{3;3,1,1}$

$S_{2;3,1,1}$ or $S_{1;3,1,1}$
and \( \sigma = \sum_{m=-3}^{2} m \sqrt{12 - m(m + 1)}|\psi_{m+1}^{*}\psi_m| \). Removing spin-independent terms, the energy becomes \( E = N\beta / 2 \), with
\[
\epsilon = \tilde{p} f_{c} + \tilde{c}_{1} f_{c}^{2} + \frac{4c_2}{7} |s_{-}|^{2} + c_3 \left( \frac{3\gamma_z^2}{2} - 12 \gamma_z + \frac{|\eta|^2}{2} + 2|\sigma|^2 \right),
\]
where \( \tilde{p} = 2p / N \beta \), and \( \tilde{c}_1 = c_1 - c_3 / 2 + \sqrt{16\pi / \beta} c_d / \beta \). Since \( c_d \ll c_1 \), dipolar effects are not relevant for the equilibrium discussion. We will hence set \( \Gamma_0 = 0 \).

We have minimized Eq. (4) with respect to \( \psi_m \), under the constraints \( \sum_m |\psi_m|^2 = 1 \) and \( f_+ = 0 \) [29]. Figs. 4 shows the corresponding phase diagram, which although in basic agreement with that worked out recently in Ref. [29] presents certain differences in its final form. For the phases discussed below \( \sigma = 0 \) [27]. For sufficiently negative \( g_0 \) the system is in a polar phase \( P = (c\theta, 0, 0, 0, 0, 0, s\theta) \), where \( c = \cos \), and \( s = \sin \). This phase is characterized by \( f_{c} \approx \tilde{p} / \tilde{p}_c \left( p_c \approx 6\tilde{c}_1 \approx 0.36, \right) 4|s_{-}|^{2} = 1 - \tilde{p}^{2} / \tilde{p}_c^{2} \), \( \gamma_z \approx 9 \), and \( |\eta| \approx 0 \). The polar phase extends up to \( g_0 / g_6 = 0.01 \) for \( p = 0 \). For sufficiently large \( g_0 \) and \( \tilde{p} \), \( CY_{-3,2} = (c\theta, 0, 0, 0, 0, s\theta, 0) \) occurs. This phase is cyclic \( (s_{-} = 0) \) and it is characterized by \( f_{c} \approx \tilde{p} / \tilde{p}_c \left( p_c \approx 6\tilde{c}_1 \approx 0.36, \right) \). Both \( p \) and \( CY_{-3,2} \) continuously transform at \( \tilde{p} = \tilde{p}_c \) into a ferromagnetic phase \( F = (c\theta, 0, 0, 0, 0, 0, 0) \). For \( 0.04 < \tilde{p} < 2\tilde{c}_1 \) and \( CY_{-3,2} \) becomes degenerated with the cyclic phase \( CY_{-1,2} = (c\theta, 0, 0, 0, 0, 0, s\theta, 0) \). The latter state differs from \( CY_{-3,2} \), since \( \gamma_z = 2 - \tilde{p}^{2} / \tilde{p}_c^{2} \). For sufficiently large \( g_0 \) and \( \tilde{p} < 0.04 \), a cyclic phase \( CY_{-1,3} \) of the form \( (\psi_{-3,0,0,\pm 1}, \psi_{-1,1,3}) \) of the form \( (\psi_{-3,0,0,\pm 1}, \psi_{-1,1,3}) \) occurs. Contrary to the other phases this cyclic phase is characterized by \( |\eta| > 0 \) [29]. Finally for a region around \( g_0 = 0 \) another phase with \( |\eta| > 0 \), \( |s_{-}| > 0 \) is found. In this phase two possible ground states are degenerated [29], namely \( S_{-2,0,2} = (0, 0, \psi_{-1,0,0,\pm 1}, \psi_{-1,0,0,\pm 1}) \), and \( S_{-3,1,1,3} \), which has a similar form as \( CY_{-3,1,1,3} \).

For a Cr-HEC in a spherical trap frequency \( \omega \) in the Thomas-Fermi regime, \( \tilde{p} = \tilde{p}_c \) for a magnetic field (in mG) \( B \approx 1.25 \left( N / 10^5 \right)^{2/5} \left( \omega / 10^5 \times 2\pi \right)^{6/5} \). Hence, most probably, magnetic shielding seems necessary for the observation of non-ferromagnetic ground-state phases. We would like to stress as well, that there are still uncertainties in the exact values of \( a_{2,4,6} \). In this sense, we have checked for \( a_{6} = 98a_{5}, a_{4} = 64a_{5} \), and \( a_{2} = -27a_{5} \), that apart from a shift of 0.2 towards larger values of \( g_0 / g_6 \), the phase diagram remains qualitatively the same.

In the last part of this Letter, we consider the spinor dynamics within the MF approximation, but abandoning the SMA. The equations for the dynamics are obtained by deriving the MF Hamiltonian with respect to \( \psi_m(r) \):
\[
\frac{\hbar}{\partial t} \psi_m(r) = \left[ -\frac{\hbar^2 \nabla^2}{2M} + U_{\text{trap}} + pm \right] \psi_m + N \left[ \epsilon_0 n + mc_1 f_1 + c_d A_0 \right] \psi_m
\]
\[
+ \frac{N}{2} [c_1 f_2 + 2c_d A_1] S_{m,m+1}^+ \psi_{m+1}^* - \frac{N}{2} [c_1 f_2 + 2c_d A_1] S_{m,m+1}^- \psi_{m+1}^*
\]
\[
+ (-1)^m \frac{2Nc_2}{7} s \psi_{m+3}^* - \frac{Nc_3}{7} \sum_{i,j} O_{ij} (S_i S_j)_{m,n} \psi_n,
\]
where \( A_0 = \sqrt{6\pi / 5} [1 / \sqrt{8\pi} \Gamma_{0,2} + \Gamma_{1,1} + \Gamma_{-1,1}], A_{\pm} = \sqrt{6\pi / 5} [\Gamma_{0,2} / \sqrt{6} + \Gamma_{\pm 2} + \Gamma_{\pm 2} + \Gamma_{\pm 2}], \Gamma_{m,i} = \int d\mathbf{r} d\mathbf{r}^* Y_{2m}^{\pm}(\mathbf{r} - \mathbf{r}^*)/|\mathbf{r} - \mathbf{r}^*|^3 \), and \( S_{m,m+1} = \sqrt{12 / m(m+1)} \). Note that all \( \psi_{m,n}, f_i, O_{ij}, \) and \( A_i \) have now a spatial dependence. We first consider \( p = 0 \), and discuss on \( p \neq 0 \) below. There are two main features in the spinor dynamics in Cr-HEC which are absent (or negligible) in other spinor BECs. On one side the \( c_3 \) term allows for jumps in the spin manifold larger than one, and hence for a rapid dynamics from e.g. \( m = 0 \) to \( m = \pm 3 \). On the other side, the dipolar terms induce an EH-like transfer of spin into CM angular momentum.

![FIG. 2: $|\psi_{m=-3}(\mathbf{r})|^2$ at \( \omega t = 40 \) (a) and 120 (b) for \( p = 0 \), \( g_0 = 0, \omega_3 = 1kHz, N = 10^4 \) atoms, and \( \psi(t=0) = \psi_{m=-3} \). The x and y axes are in \( \sqrt{\hbar / m \omega} \) units.](image_url)

We consider for simplicity a quasi-2D BEC, i.e. a strong confinement in the \( z \)-direction by a harmonic potential of frequency \( \omega_z \). Hence \( \psi_m(r) = \phi_0(z) \psi_m(\rho) \), where \( \phi_0(z) = \exp[-z^2 / 2l_z^2 / \pi^{1/4} \sqrt{l_z}] \), with \( l_z = \sqrt[4]{\hbar / m \omega_z} \). We have then solved the 2D equations using Crank-Nicholson method, considering a harmonic confinement of frequency \( \omega \) in the \( xy \)-plane. In 2D, \( \Gamma_{\pm 1,2} = 0 \), but these terms vanish also in 3D due to symmetry, and hence the 2D physics is representative of the 3D one. The vanishing of \( \Gamma_{\pm 1,2} \) is rather important, since if \( \psi(t=0) = \psi_{m=\pm 3} \), \( \Gamma_{\pm 1,2} \) is responsible for a fast dipolar relaxation (for \( \omega t \approx 1 \)). Hence, a BEC with \( \psi(t=0) = \psi_{m=\pm 3} \) does not present any significant fast spin dynamics. However significant spin relaxation appears in the long time scale, due to the \( \Gamma_{-1,2} \) terms. This is the case of Fig. 2 where we have \( \psi(t=0) = \psi_{m=-3} \).

One of the most striking effects related with spin relaxation is the transference of spin into CM angular momentum, which resembles the famous EH effect [24]. The analysis of this effect motivated us to avoid the SMA in
the study of the spinor dynamics. In Figs. 2 we show snapshots of the spatial distribution of the $m = -2$ component. Observe that the wavefunction clearly loose its polar symmetry, since spin is converted into orbital angular momentum. The spatial patterns become progressively more complicated in time.

The other special feature of Cr-BEC, namely the appearance of the $c_3$ term can have significant qualitative effects in the dynamics both for short and for long time scales. The evolution at long time scale may present in-between or sequential population as for $F_s$ scales a jump to the extremes (the population of $\pm F$ to the case of $0$). This large jump is absent if $c_3 = 0$, and depends on the value of $g_0$. In particular, if $g_0 = 0$ one obtains at short time scales a sequential population as for $F = 2$ $^{87}$Rb.

We finally comment on the dynamics if $p \neq 0$. In the case of $F = 1$ or $F = 2$ $^{87}$Rb, the dynamics is independent of $p$ since the linear Zeeman effect may be gauged out by transforming $\psi_m \rightarrow \psi_m e^{ipm/\hbar}$, due to the conservation of the total spin. In Cr-BEC the situation is very different, since the $\Gamma_{1,2}$ do not conserve the total spin, and hence oscillate with the Larmor frequency $\omega_L = p/\hbar$ and $2\omega_L$, respectively. If $\omega_L >> \omega$ one may perform rotating-wave approximation and eliminate these terms. Hence the coherent EH-like effect disappears for sufficiently large applied magnetic fields.

In conclusion, spin-3 Cr-BEC is predicted to show different types of spin phases depending on $a_0$ and the magnetic field. The spinor dynamics also presents novel features, as a fast transference between $\psi_0 \rightarrow \psi_{\pm 3}$, and the Einstein-de Haas-like transformation of spin into rotation of the different components due to the dipole interaction.

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FIG. 3: Population of $\psi_{0,1,2,3}$ versus $\omega t$ for $g_0 = g_6$, $p = 0$, and $\psi(0) = \psi_0$. Note the rapid growth of $m = \pm 3$ (arrow).

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[26] For every $g_0$ and $p$ we performed up to 2000 different runs of a simulated annealing method to avoid the numerous local minima.
[27] We also found numerically states (similar to the Z states of Ref. [22]) with tiny $\sigma$, which are however very slight variations of neighboring phases, with which they are in practice degenerated.
[28] $|\eta| \neq 0$ leads to the interesting possibility of biaxial nematics, as recently pointed out for the first time in
Ref. [23].

[29] These phases are degenerated for any practical purposes, with relative energy differences $< 0.01\%$. A small seed in the other components triggers the mean-field evolution.

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