Spin-thermodynamics of cold spin-1 atoms decoupled from spatial modes

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We study the thermodynamic properties of cold spin-1 atoms with a fixed magnetization \( M \) and decoupled from spatial modes. Three temperature domains are found: (0, \( T_1 \)) is a domain of second condensation, namely, both the spatial and spin degrees of freedom are frozen; (\( T_1, T_2 \)) is a \( T \)-sensitive domain, where the internal energy \( U \propto T \), entropy \( S_E \propto \log T \), and \( U/k_B T \) is always less than 3/2; (\( T_2, T_3 \)) is the third domain with a maximum entropy. When \( T \) is higher than \( T_3 \), the spatial modes can not be neglected. The appearance of these domains originates from the two gaps: (i) The gap between the ground state and the first excited state, and (ii) the gap between the highest spin-state without spatial excitation and the lowest state with a spatial mode excited. These two gaps are crucial to the low temperature physics and they can be tuned.

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Since the pioneering experiment on spinor condensation \( 1 \), the study of these artificial and tunable systems becomes a hot topic \( 1 \). Due to the rapid development of low-temperature techniques \( 9–12 \), a magnificent goal becomes a hot topic \( 1–8 \). Due to the rapid development of low-temperature techniques \( 9–12 \), a magnificent goal becomes a hot topic \( 1–8 \). Due to the rapid development of low-temperature techniques \( 9–12 \), a magnificent goal becomes a hot topic \( 1–8 \). Due to the rapid development of low-temperature techniques \( 9–12 \), a magnificent goal becomes a hot topic \( 1–8 \). Due to the rapid development of low-temperature techniques \( 9–12 \), a magnificent goal becomes a hot topic \( 1–8 \). Due to the rapid development of low-temperature techniques \( 9–12 \), a magnificent goal becomes a hot topic \( 1–8 \).
or they vary oppositely if \( c > 0 \). Moreover, we have \( \frac{∂S}{∂e} = C/T \) and \( \frac{∂S}{∂c} = -C/c \). Thus the increasing of \( T \) always leads to an increase of \( S_E \), while the increasing of \( |c| \) always leads to a decrease of \( S_E \). In particular, Eq. (2) relates the three thermodynamic functions to each other, \( U = TC + cY \).

Numerical examples are shown in Fig. 1, where the realistic parameters of interaction are used. The variation of thermodynamic functions versus \( T \) shows three steps: insensitive, sensitive, and insensitive again. For example, the \( U \) of Rb and Na remains to be zero when \( T \) is very low. Once \( T \) is higher than a turning point \( T_1 \), a sudden increasing of \( U \) happens (as shown in Fig.1a). When \( T \) is higher than the second turning point \( T_2 \), \( U \) does not increase any more and remains \( \approx |cN_U| \). Note that the energy gap between the g.s. and the first excited state is \( E_{gap,1} = |c|(2N - 1) \) (if \( c < 0 \)) or \( = |c|(2M' + 3) \) (if \( c > 0 \)). Thus, when \( M' \) is small, the gap for Rb is much larger than the gap for Na. On the other hand, we find \( T_1 \) for Rb is much larger than the one for Na from Figs. 1a and 1e. Therefore, a larger gap might lead to a higher \( T_1 \). Furthermore, for Na, among the three curves in Fig. 1e with different \( M \), the dotted curve with \( M = 1500 \) has the largest \( T_1 \). It suggests also that a larger gap might give a higher \( T_1 \).

The domain \( (T_1, T_2) \) is a \( T \)-sensitive domain, where \( U \) increases almost linearly with \( T \) (accordingly \( C \) is close to a constant), and also \( S_E \) increases nearly linearly with \( \ln T \) disregarding \( c < 0 \) or \( c > 0 \). When \( c < 0 \), we know from Fig. 1b and 1c that the variations of \( C \) and \( Y \) are synchronous as predicted. Whereas they behave Oppositely when \( c > 0 \) as shown in Figs. 1f and 1g. It is worth to point out that the lower part of the spectrum depends (does not depend) on \( M \) if \( c > 0 \) (< 0). Therefore, all the curves in Fig. 1 for Na depend on \( M \) strongly, while those for Rb do not.

In the g.s., both the spatial and spin degrees of freedom are frozen. This can be called the second condensation \[12\]. The probabilities at the g.s. is \( P_g = 1/Z \). When \( T = 0 \), \( P_g = 1 \). When \( P_g \) decreases from 1, the spin-fluctuation begins. The probability at the highest spin-state is \( P_{top} = e^{-\beta E_{top}} /Z \), where \( E_{top} = \frac{|c|}{2}[N(N+1) - M'(M'+1)] \) is the energy difference between the highest and the lowest spin-states. Note that, in the pure spin-space, \( \lim_{T \to \infty} P_{top} \to 1/N_{state} \). Thus

### TABLE I: The boundary conditions for thermodynamic functions

| \( U \) | \( C \) | \( Y \) | \( S_E/k_B \) |
|-------|-----|-----|-------------|
| \( T \to 0 \) | 0 | 0 | 0 |
| \( T \to \infty \) | \( |cN_U| \) | \( N_U \) | \( \ln N_{state} \) |
| \( c \to 0 \) | 0 | 0 | \( N_U \) | \( \ln N_{state} \) |
| \( c \to \infty \) | 0 | 0 | 0 |

The deviation of \( P_{top}N_{state} \) from 1 measures how far the spin-fluctuation is away from the maximum value. Examples of \( P_g \) and \( P_{top}N_{state} \) are shown in Fig. 2. To show the \( T \)-sensitivity, \( U/k_B T \) and \( C/k_B \) are also plotted. It is found that \( T_1 \) is the position that \( P_g \) starts to decline from 1. Thus \( T_1 \) marks the temperature of the second condensation. \( T_2 \) is the place that \( P_{top}N_{state} \) starts to decrease from 1. Thus \( T_2 \) marks the maxima of spin-fluctuation and entropy. To describe it quantitatively, \( T_1 \) and \( T_2 \) are defined at which \( P_g = 0.95 \) and \( P_{top}N_{state} = 0.95 \), respectively. When \( T \) is very low, \( P_g \) can be approximated by \( P_g = \frac{1}{1 + e^{-\beta E_{gap,1}/k_B}} \), and accordingly \( T_1 = 0.34 E_{gap,1}/k_B \).

Furthermore, our calculation demonstrates that \( U/k_BT \) is always less than 3/2 as shown in Fig. 2. It implies that, disregarding \( N \) and interactions, the internal energy contributed from all the spin degrees of freedom is even smaller than the energy assigned to the spatial motion for a single particle. This fact manifests how small the energy is involved in the spin-space.

Let the energy of the lowest state with a spatial mode excited be \( E_{ex}^{c} \), which can be obtained by solving the equation given in the ref. \[19, 20\]. How weak the interference from the spatial mode would be depends on the gap \( E_{gap} = E_{ex}^{c} - E_{top} \). When the gap is sufficiently large, the probability of staying in the spatially excited levels is negligible. The temperature at which \( e^{-\beta E_{gap,2} = 0.05} \) is defined as \( T_3 \) (i.e., \( T_3 = \frac{E_{gap,1}}{\beta k_B} \)). When \( T < T_3 \), the spin-space is decoupled from the spatial modes.

When both \( N \) and \( M \) are fixed, the dependence of \( T_1, T_2, \) and \( T_3 \) on \( \omega \) is shown in Fig. 3. Note that a larger \( \omega \) will lead to a more compact \( \phi(r) \) (smaller in size) and thereby a stronger \( |c| \). Hence, all the \( T_1, T_2 \) and \( T_3 \) will become higher when \( \omega \) increases. For Rb, the second condensation can be realized at \( T_1 = 10^{-9}K \) when \( \omega = 10^{4.5}s^{-1} \) and \( N = 1000 \)(Fig.3a). If \( \omega \) and/or \( N \) are larger, \( T_1 \) is even higher. For Na, \( E_{gap,1} \propto M' \), therefore \( T_1 \) depends on \( M \) seriously. When \( M = N - 2 \) and \( N = 1000 \), \( T_1 \) would be higher than \( 10^{-9}K \) if \( \omega > 10^{5.7}s^{-1} \) (3c).

When \( N \) is small \( T_3 \) can be quite high (say, \( T_3 > 10^{-8}K \) if \( \omega > 10^{4}s^{-1} \) (3b,3d). It implies that a nearly pure spin-system can be created experimentally. When \( N \) is larger, due to the cross over of the highest member of the ground band and the lowest member of the excited band, \( T_3 \) does not exist unless \( M \) is close to \( N \) (3a and 3c). In 3a (3c) and when \( \omega = 10^{2-1}s^{-1} \) (10^{2-28}s^{-1} \), a cross over of \( T_3 \) and \( T_2 \) occurs. When \( \omega \) is smaller than the value, the domain \( (T_1, T_2) \) is under \( T_3 \) so that the whole process of the increase of entropy from zero to being maximized is free from the interference of the spatial modes.

Since the thermodynamic functions change greatly in the \( T \)-sensitive domain, the spin-texture and spin-component \( \mu \) should be modulated accordingly. For \( \phi^N_{SM} \), the probability of a particle in \( \mu \) can be calculated from
Eq. (10) in Ref. [21]. In particular, when $\mu = 0$ the probability is

$$P_0^{SM} = \frac{S(S+1)(2N+1) - M^2(2N+3) - N}{N(2S+3)(2S-1)}$$

(4)

When the thermo-fluctuation is taken into account, we define

$$\mathcal{P}_0^M(T) = \frac{1}{Z} \sum_{S} P_0^{SM} e^{-\beta E_S}$$

(5)

and the population of $\mu = 0$ component is $N\mathcal{P}_0^M(T)$. Examples of $\mathcal{P}_0^M(T)$ are given in Fig. 4. When $T \to 0$ and for Rb, $\mathcal{P}_0^M(0) = P_0^{SNM} = \frac{N^2 - M^2}{N(2N-1)}$, while for Na, $\mathcal{P}_0^M(0) = P_0^{SNM} = \frac{N^2 - M}{N(2N+1)}$. In both cases, $\mathcal{P}_0^M(0)$ decreases with $M$. As $T$ increases, $\mathcal{P}_0^M(T)$ remains unchanged until $T$ enters into the $T$-sensitive domain. Thus the borders of the $T$-sensitive domain can be evaluated by measuring $\mathcal{P}_0^M(T)$.

When a magnetic field $B$ is applied, the linear Zeeman term can be dropped for the $M$-conserved systems, the quadratic Zeeman term corresponds to $H_B = q \sum_{i} f_{iz}$, where $f_{iz}$ is the $z$-component of the spin-operator for the $i$-th particle. Under $H_B$, the states with different $S$ will mix up, and the $i$-th eigenstates will appear as $\Psi_{iM}^B = \sum_{S} C_{iS}^{B} \Psi_{SM}$. The matrix elements $\langle \delta_{SM} | H_B | \delta_{SM} \rangle$ are shown in Eqs. (3,4,6,7) of Ref. [21]. By diagonalizing the matrix of $H + H_B$, the eigenvalues $E_{i}^B$ and $\Psi_{iM}^B$ can be obtained. It is found that there is always a turning point $B_0$ so that the spectra will remain nearly unchanged when $B \leq B_0$ as shown in Fig. 5, where $B_0 = 0.5 mG$. Based on the perturbation theory $\Psi_{iM}^{B+\varepsilon}$ would be closer to $\Psi_{iM}^{B}$ (where $\varepsilon$ is a small quantity) if the levels in the neighborhood of $E_{i}^{B}$ are wider separated. Accordingly, the $B_0$ for Rb is much larger than that for Na because the low-lying levels of the former are much splitting. Furthermore, a smaller $N$ can lead to a larger $\int |\phi(r)|^2 dr$, therefore a larger $|c|$ and accordingly a larger level-separation resulting also in a larger $B_0$. For Na, the level-separation depends on $M$, hence a larger $M$ will also lead to a larger $B_0$. Since all the thermodynamic properties depend solely on the spectra, the invariance of the spectra implies that all the features at $B = 0$ will remain unchanged when $B \leq B_0$.

In summary, the $M$-conserved pure spin-systems of cold Rb and Na atoms at $B = 0$ are studied, three domains of $T$ are found. The effect of a residual $B$ has been evaluated. The main results are:

1) $(0, T_1)$ is a $T$-insensitive domain originated from the gap $E_{gap,1}$, and $T_1 = 0.34 E_{gap,1}/k_B$ marks the second condensation [12]. It is reported (Fig. 2 of Ref. [12]) that, for a spin-3 condensation, $M$ depends on $T$ in general, but becomes insensitive to $T$ when $T \to 0$ and $B$ is sufficiently weak. Thus, the appearance of the $T$-insensitive domain during $T \to 0$ might be a common phenomenon.

2) $(T_1, T_2)$ is a $T$-sensitive domain, where the thermo-fluctuation keeps strengthening. $U \propto T$ and $S_E \propto \ln T$ roughly hold, and $U/k_BT < 3/2$ holds. The location of this domain can be known by measuring $\mathcal{P}_0^M(T)$.

3) $(T_2, T_3)$ is again a $T$-insensitive domain with $T_3 = \frac{E_{gap,2}}{3k_B}$. Due to the gap $E_{gap,2}$, the excitation of spatial modes is suppressed.

4) Both $E_{gap,1}$ and $E_{gap,2}$ can be tuned by changing $\omega$, $N$, and $M$. Correspondingly, $T_1$, $T_2$, and $T_3$ also change. A larger $N$ (for Rb) or a larger $|M|$ (for Na) will lead to a larger $E_{gap,1}$ and the second condensation can be realized at higher temperature. The domain $(T_1, T_2)$ can be compressed by reducing $E_{top}$ (i.e., by increasing $M$). In particular, the low-dimensional systems are notable for application. For example, a 2-level system can be formed by fixing $M = N - 2$.

5) The present techniques can provide a shield so that the effect of a residual $B$ is negligible. On the other hand, when $B$ is stronger, its effect should be studied further.

6) It is also possible to consider an optical-lattice (OL) potential, or maybe an HP-OL combination. In that case, a deep OL may additionally freeze the spatial mode to realize the pure spin-system.

As a final remarks, the two gaps $E_{gap,1}$ and $E_{gap,2}$ are in general crucial to the physics at $T < T_c$.

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FIG. 1: (Color online). log $U$, C, log $|Y|$, and $S_E$ of Rb (left column) and Na (right column) condensates versus log$_{10}T$. The unit of $U$ is $\hbar \omega$. $N = 3000$ and $\omega = 300 \times 2\pi$ are assumed. $M$ is given at 0 (solid line), 500 (dash), and 1500 (dot). For (c) and (e), the sign of $Y$ is marked by the curves.

FIG. 2: (Color online). Six functions of Rb (a) and Na (b) versus log$_{10}T$. Curve “1” is for $U/k_B T$, “2” is for $C/k_B$, “3” is for $P_g$, “4” is for $P_{g,app}$, “5” is for $P_{top,N_{state}}$, and “6” is for $P_{top,ap,N_{state}}$. ($P_{top,ap}$ is obtained by transforming the summation involved into an integration). $N = 3000$, $M = 0$, and $\omega = 300 \times 2\pi$ are used.
FIG. 3: (Color online). $T_1, T_2$ and $T_3$ versus $\omega$. Solid lines are for $M = N - 2$, dash for $M = 0$. When $M = 0$ and $N = 1000$, $T_3$ does not exist.

FIG. 4: (Color online). $P_0^M(T)$ versus $T$ for Rb (a) and Na (b). The parameters and the three choices of $M$ are the same as in Fig. 1.
FIG. 5: (Color online). The spectrum of a Na condensate versus $B$. The lowest ten curves are plotted.