Quantum phase transition in an atom–molecule conversion system with atomic transition

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Abstract
The quantum phase transition in an atom–molecule conversion system with atomic transition between two hyperfine states is studied. In the mean-field approximation, we give the phase diagram in which the phase boundary only depends on the atomic transition strength and the atom–molecule energy detuning, but not on the atomic interactions. Such a phase boundary is further confirmed by calculating the fidelity of the ground state and the energy gap between the first excited state and the ground state. As a comparison to the mean-field results, we also study the quantum phase transition with the full quantum method where the phase boundary depends on the particle number. Analysing the finite-size scaling behaviours of the energy gap, the fidelity susceptibility and the first-order derivative of entanglement entropy with respect to the atomic transition strength, we obtain their critical exponents by numerical calculation and show that in the thermodynamic limit, one can obtain the same phase boundary as in the mean-field approximation. Our results show a new way to manipulate the quantum phase transition by regulating the atomic transition strength with the intensity of the laser.

(Some figures may appear in colour only in the online journal)

1. Introduction
Quantum phase transition describes an abrupt change in the ground state of many-body systems as some system parameter is tuned across a critical point at zero temperature. There have already been extensive studies of quantum phase transition in the quantum Hall systems [1], the superconductors [2], etc. Now the ultracold atomic systems, especially the Bose–Einstein condensates, provide us another flexible platform to observe and study the quantum phase transition [3]. The experiment by Bloch et al on ultracold atoms in an optical lattice has given us a perfect example of the quantum phase transition from a superfluid to a Mott insulator [4], which brought on lots of similar studies [5, 6]. Other quantum phase transitions, such as the transition between non-entangled and entangled states in the two-mode Bose–Einstein condensates [7], between degenerate and non-degenerate ground states in the extended bosonic Josephson junction model [8], and between a pure molecule (PM) state and a mixed atom–molecule (AM) one in an AM model [9–13], have also been investigated. Note that in the earlier AM model, one mainly controlled the quantum phase transition by tuning the energy detuning between the atomic and the molecular states.

Molecular Bose–Einstein condensates are versatile in physical studies because, in comparison to atomic Bose–Einstein condensates, they offer more degrees of freedom to manipulate. For example, the ultracold polar molecules have been used to study the ultracold chemistry and quantum information science. The polar molecules with nonzero dipole moments may be either heteronuclear [14–17] or homonuclear. One extensively discussed example of the latter is the Rydberg molecules which were created by Pfau et al in experiments for the first time [18] and then studied widely [19–21]. One Rydberg molecule consists of two atoms which are in different states, such as the ground and Rydberg states. The atomic transition between these two hyperfine states can be realized through a two-photon process, which may provide a new control parameter, i.e., the atomic transition strength, for
the quantum phase transition. The quantum phase transition between a PM state and a mixed AM state in an AM conversion system without the atomic transition has just been studied [9–13]. Then a natural question arises concerning the effect of the atomic transition between two different hyperfine states on the quantum phase transition.

In this paper, we study the influence of the atomic transition on the phase transition of an AM conversion system in the mean-field approximation (MFA) and with the full quantum method. It is interesting to note that we can still observe the phenomenon of the phase transition when the energy detuning is tuned, even if the AM energy detuning is fixed on a certain value, which is different from the pure AM conversion system as discussed in [12]. The quantum phase transition between a PM state and a mixed AM state can be controlled with the energy detuning, which can be realized by tuning the magnetic field in a magnetic Feshbach resonance or the frequency of the laser in photoassociation, so far as we know. While the atomic transition strength can be tuned by varying the intensity of the laser which is more convenient than varying the frequency of the laser, which may provide us a good avenue to control the phase transition. We show the detailed phase diagram in the MFA, whose phase boundary can also be confirmed by the full quantum calculation in the thermodynamic limit (i.e., $N \to \infty$). The finite-size scaling behaviours of the energy gap, fidelity susceptibility and the first-order derivative of entanglement entropy with respect to the atomic transition, are also discussed to support the same conclusion.

In the following section, we give the model of the system and the general phase diagram in the MFA. The energy gap and fidelity are also studied to characterize the phase transition. In section 3, we study the quantum phase transition from a PM state to a mixed AM state with the full quantum method. The energy gap, the fidelity susceptibility, the entanglement entropy, and the first-order derivative of entanglement entropy with respect to the atomic transition strength, together with their finite-size scaling behaviours and analyses, are thoroughly investigated. In the last section, we give a brief summary and discussion.

2. Model and phase diagram

We consider the AM conversion system where one molecule is composed of two atoms residing in two different hyperfine states, respectively. Additionally, we assume that the atoms can transit between the two hyperfine states. The corresponding Hamiltonian reads

$$H = -J(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i) + \frac{\delta a}{2}(\hat{a}_{i+1}^\dagger \hat{a}_{i+1} - \hat{a}_i^\dagger \hat{a}_i)
+ \frac{U}{2}(\hat{a}_i^\dagger \hat{a}_i \hat{a}_{i+1}^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_{i+1} \hat{a}_i^\dagger \hat{a}_i)
+ g(\hat{b}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{b}_i + \hat{b}_i + \hat{a}_i^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_i),$$  \hspace{1cm} (1)

where $\hat{a}_i$ (i = 1, 2) annihilates (creates) an atom in the i-th hyperfine atomic state and $\hat{b}_i$ ($\hat{b}_i^\dagger$) annihilates (creates) a molecule. Here $J$ refers to the atomic transition strength between the two hyperfine states and $U_a$ ($U_a^\prime$) the strength of atomic intracomponent (intercomponent) interaction. We have ignored the molecular interactions for the sake of simplicity. $g'$ is the AM coupling strength, $\delta a$ is the energy detuning between the two hyperfine atomic states and $\delta b$ is the energy detuning between the atomic and molecular states.

In order to study the property of the system we considered, the dynamical equations are desired. In the MFA, the Heisenberg equations of motion for the operators $\hat{a}_i$ (i = 1, 2) and $\hat{b}$ can be easily converted into their mean-field version by replacing the operators with their average values, i.e., $a_i \approx \langle \hat{a}_i \rangle / \sqrt{N}$, $\alpha_2 \approx \langle \hat{a}_2 \rangle / \sqrt{N}$ and $\beta \approx \langle \hat{b} \rangle / \sqrt{N}$. Here $N = \langle \hat{a}_1^\dagger \hat{a}_1 \rangle + \langle \hat{a}_2^\dagger \hat{a}_2 \rangle + 2\langle \hat{b} \hat{b} \rangle$ is the total particle number. Due to the conservation of the total particle number, $|\alpha_1|^2 + |\alpha_2|^2 + |\beta|^2 = 1$ is required in the MFA. We may further assume $\alpha_1 = \sqrt{\rho_1^{\prime} e^{\phi_1}}$, $\alpha_2 = \sqrt{\rho_2^{\prime} e^{\phi_2}}$ and $\beta = \sqrt{\rho_0 e^{\phi_0}}$, where $\rho_i$ and $\phi_i$ (i = 1, 2) refer to the atomic/molecular populations and phases, respectively. The conservation law of total particle number now reads $\rho_1 + \rho_2 + 2\rho_0 = 1$. Therefore, the mean-field dynamical equations of the system can be written as

$$\dot{\rho}_a = \left[ J \cos(2\phi_a) - g(\sqrt{\rho_a} e^{\phi_a}) - \frac{U}{2} - U^\prime \right] + \delta a/2, \hspace{1cm} \phi = \left[ \frac{2J \cos(2\phi_a) - 2g(\sqrt{\rho_a} e^{\phi_a})}{\sqrt{(1 - 2\rho_a)^2 - z^2}} - U - U^\prime \right] (1 - 2\rho_a) + \frac{g}{2}\sqrt{(1 - 2\rho_a)^2 - z^2} \rho_a \cos \phi + \frac{3\delta b}{2},$$

$$\dot{z} = -2J(1 - 2\rho_a)^2 - \frac{z^2}{\rho_a} \sin(2\phi_a), \hspace{1cm} \rho_b = g\sqrt{(1 - 2\rho_a)^2 - \frac{z^2}{\rho_a} \sin \phi},$$

where $\phi_a = (\theta_2 - \theta_1)/2$, $\phi = \theta_1 + \theta_2 - \theta_b$ and $\rho_a = g\sqrt{(1 - 2\rho_a)^2 - \frac{z^2}{\rho_a} \sin \phi}$ describe the phase and population differences, respectively. Here, the rescaled parameters are $U = NU_a$, $U^\prime = NU_a^\prime$ and $g = \sqrt{Ng'}$. The Hamiltonian canonical equations, i.e., $\dot{\rho}_a = \partial H_M^a / \partial z$, $\dot{z} = -\partial H_M^a / \partial \phi_a$, $\phi = \partial H_M^a / \partial \rho_b$ and $\dot{\rho}_b = -\partial H_M^a / \partial \phi$ have been satisfied in (2), where the Hamiltonian in the MFA reads

$$H_{MB} = -J \sqrt{(1 - 2\rho_a)^2 - z^2} \cos(2\phi_a) + \frac{\delta a}{2} z
+ \frac{U}{4}[1 - 2(1 - 2\rho_a)^2 - z^2] + \frac{U^\prime}{4}[1 - 2(1 - 2\rho_a)^2 - z^2]
+ g\sqrt{(1 - 2\rho_a)^2 - z^2} \rho_a \cos \phi + \frac{\delta b}{2}(3\rho_b - 1).$$  \hspace{1cm} (3)

As we know, the fixed points correspond to the eigenvalues of the nonlinear system [22]. We may study the static property of the system by solving the fixed points which require $\phi_a = 0$, $\phi = 0$, $z = 0$ and $\rho_b = 0$. Many fixed point solutions may be expected. In the following discussion, we only focus on the fixed points with $z = 0$ since they contain the ground and the first excited states. Such fixed points read

$$\rho_b = \left[ \Delta + \sqrt{\Delta^2 + 6g^2 \cos \phi} \right] \rho_{\alpha_0} \sin(2\phi), \hspace{1cm} \phi = 0(\pi), \hspace{1cm} 2\phi_a = 0(\pi),$$

where $\Delta = 3\delta_b/2 + 2J \cos(2\phi_a)$ is defined. The solutions (4) are obtained by assuming $\delta_a = 0$ and $U = U + U^\prime = 0$. Note that for the case of $U \neq 0$, we cannot obtain the analytical
solutions of the fixed points. However, by numerical means, we find that the nonzero $U$ does not change the phase boundary between the PM and the mixed AM phases, as we are going to discuss in the following.

In figure 1(a), we plot the dependence of molecule population $\rho_b$ on the transition strength $J$ for the ground and first excited states. The three quantities in the legend of the figure denote the values of $\tilde{U}$, $2\theta_b$ and $\phi$, respectively. The lines with $(\tilde{U},0,\pi)$ correspond to the ground states for different $\tilde{U}$, and the line with $(0,\pi,\pi)$ corresponds to the first excited state for $\tilde{U}=0$. Note that $\rho_b$ of the first excited state shows no sensitivity to the value of $\tilde{U}$, so the line with $(0,\pi,\pi)$ can also denote the first excited state for different interaction strengths. From figure 1(a), we can find that the ground state is a PM state ($\rho_b=0$, $\rho_b=0.5$) when $J<J_c$, and it is a mixed AM state ($\rho_b\neq0$, $\rho_b\neq0$) when $J>J_c$, where $J_c=(3-\sqrt{2})g/2$ with $\delta_b=-2g$. The general phase diagram of the ground state in the parameter space of $\delta_b$ and $J$ is given in figure 1(b), from which we can determine the value of $J_c$ by locating the boundary between the PM and the mixed AM phases which satisfies $3\delta_b/2+2J_c=-\sqrt{2}g$. Note that for the case of $J=0$, the critical point $\delta_c=-\sqrt{8/9}g$ agrees well with the result in [12]. Additionally, as seen in the general phase diagram, the phase transition can be controlled with the atomic transition strength as well as the energy detuning, which can be realized with different experimental methods.

In order to further confirm the phase boundary, we show in figure 2 the dependence on $J$ of the energy gap $\Delta E_{MF}$ between the first excited state and the ground state, and of the fidelity of the ground state in the mean-field approximation (MFA), marked with the blue dashed line and the green solid line, respectively. The parameters are $\delta_b=-2g$ and $\Delta J=0.001g$.

Figure 1. (a) The population of molecules $\rho_b$ versus the transition strength $J$ for the ground and first excited states with different interactions. The parameter is $\delta_b=-2g$. (b) The mean-field phase diagram of the ground state in the parameter space of $\delta_b$ and $J$. The pure molecule (PM) phase and the mixed atom–molecule (AM) phase are separated by a critical line (marked with the blue solid line).

Figure 2. Atomic transition strength $J$ profiles of the energy gap between the first excited state and the ground state $\Delta E_{MF}$ and of the fidelity of the ground state in the mean-field approximation (MFA), marked with the blue dashed line and the green solid line, respectively. The parameters are $\delta_b=-2g$ and $\Delta J=0.001g$.

3. Quantum phase transition

We are more interested in the quantum version of the above phase transition. To this end, we need to adopt the full quantum method. For a finite particle number $N$, we may choose the Fock bases $|n,N-n-2m,m\rangle$ $(n \in [0,N], m \in [0,N/2], N-n-2m \geq 0)$ to expand the system states. Here $n$ is the number of atoms in the first atomic hyperfine state and $m$ is the number of molecules. The dimension of such bases is $(N/2+1)^2$. For convenience, the form of the Fock bases is

$$|n\rangle = \frac{1}{\sqrt{n+1}} \sum_{m=0}^{\lfloor n/2 \rfloor} \binom{n}{m} |2m\rangle.$$
simplified as $|n, m\rangle$. Then the eigenstate of the system can be written as

$$\Psi(J) = \sum_{n+2m\leq N} C_{n,m} |n, m\rangle,$$

where $C_{n,m}$ are complex coefficients dependent on the system parameters and $\sum_{n+2m\leq N} |C_{n,m}|^2 = 1$. The eigenvalues and eigenstates of the system can be easily obtained by exactly diagonalizing the Hamiltonian (1). Then the populations of the atoms and the molecules at the ground state $|\Psi_0(J)\rangle = \sum_{n+2m\leq N} C_{0,n,m} |n, m\rangle$ can be defined as $\rho_0 = \sum_{n+2m\leq N} |C_{0,n,m}|^2 (N - 2m)/N$ and $\rho_B = \sum_{n+2m\leq N} |C_{n,m}|^2 m/N$ which satisfy the relation $\rho_0 + 2\rho_B = 1$.

In figure 3, we plot the population of atoms for the ground state with the finite particle number $N$ together with the results in the MFA as a comparison. We can see that the quantum phase transition from a PM state to a mixed AM state happens as the system size increases. As the system size $N$ increases, the position of the minimum energy gap $\rho_0$ of the energy gap minimum $\rho_{min}$ converges to zero with different system sizes. From figures 4(b) and (c), we find that the critical exponent of $\rho_0$ and $\rho_{min}$ approach zero, where $\delta \rho_0 \approx 2/3$ and $\mu = 1/3$ are the critical exponents of $\rho_0$ and $\rho_{min}$, respectively. So in the thermodynamic limit, $J_c$ tends to the critical point $J_c$ and $\rho_{min}$ converges to zero.

### 3.1. Energy gap

Now we are in a position to study quantum phase transition by focusing on the energy gap which has been used to characterize the quantum phase transition [11–13, 15]. As in the mean-field calculation, here the energy gap is defined as the energy difference between the first excited state $E_1$ and the ground state $E_0$, i.e., $\Delta E = E_1 - E_0$. In figure 4(a), the energy gap $\Delta E$ is shown as a function of $J$ for different total particle numbers $N$. For a fixed energy detuning $\delta \rho_0$, the avoided level crossing between the ground and the first excited states appears at the quasi-critical point $J_c$ where the energy gap reaches its minimum $\Delta E_{min}$. As the system size $N$ increases, the position $J_c$ of the energy gap minimum $\Delta E_{min}$ gets closer to $J_c$ and the minimum amount of the energy gap $\Delta E_{min}$ decreases.

To further characterize the finite-size effect present in figure 4(a), we show the scaling behaviours of $\Delta J = J_c - J_c$ and $\Delta E_{min}$ on the particle number $N$ for different interaction strengths $U$ in figures 4(b) and (c) with power-law expressions $\Delta J \propto N^{\mu}$ and $\Delta E_{min} \propto N^{\mu}$. In two such panels, the discrete points denote the numerical results for finite particle numbers $N$, while the solid lines are the fitting functions. They show how the quantum results approach the ones in the MFA as $N$ increases, especially $N \to \infty$. From figures 4(b) and (c), we find that both $\Delta J$ and $\Delta E_{min}$ converge to zero with different system sizes and $\Delta J$ and $\Delta E_{min}$ are zero critical points. So in the thermodynamic limit, $J_c$ tends to the critical point $J_c$ and $\rho_{min}$ converges to zero. These agree well with the results in the MFA, where the minimum energy gap is zero at the critical point $J_c$. In order to illustrate the quantum phase transition, we calculate the scaling behaviour for different values of $U$. For instance, the finite-size scaling analysis of the energy gap with $U = 2g$ for different system sizes is shown in figure 4(d). According to the finite-size scaling ansatz, the rescaled energy gap around the critical point takes the form $1 - \Delta E_{min}/\Delta E = f_1(N(J - J_c))$, where $\nu$ is the correlation length critical exponent. The scaling function $f_1(x)$ should be universal and independent of the system size $N$ in this quantum phase transition. All the data of different system sizes $N = 130, 150, 170, 190, 210$ shown in figure 4(d) collapse onto a single curve as expected. It implies that the system at the critical point is scaling invariant with $\nu = 2/3$, which is the same as the correlation length critical exponent in the Lipkin–Meshkov–Glick model [23, 24]. Additionally, the critical exponent of $\Delta E_{min} \propto \mu = 1/3$ which can be estimated in the limits of both large $N (N \gg 1)$ and strong interaction $\left(\tilde{U} \gg 1\right)$. In the limit of $\Delta U \gg 1$, where the fermionization of the bosons has been proved [25], the effective energy per atom is about proportional to $N_{c}^{3/3} \left[26\right]$, and then the energy gap is the difference of two effective energies with atom numbers $N_c$ and $N_c - 2$. Therefore, in the large $N$ limit, the energy gap is proportional to $N^{-1/3}$, which agrees well with our numerical results.

### 3.2. Fidelity susceptibility

The quantum fidelity, defined as the absolute value of the overlap between two ground states with an infinitesimal variation of the control parameter, serves as another powerful tool to characterize the quantum phase transition [11, 13, 27–29]. In order to study the effect of the atomic transition strength $J$ on the quantum phase transition of the ground state, the fidelity can be written as

$$F(J, \delta J) = |\langle \Psi_0(J) | \Psi_0(J + \delta J) \rangle|,$$

where $|\Psi_0(J)\rangle$ and $|\Psi_0(J + \delta J)\rangle$ are two ground states of the system with a small parameter difference $\delta J$. We note that although the fidelity value always drops near the critical point $J_c$, its exact value depends on $\delta J$. In order to mend this deficiency, we make use of the concept of fidelity susceptibility [8, 27, 30]. In the first-order perturbation theory, we consider the atomic transition term as the perturbation term, i.e.,
The fidelity susceptibility, $\chi(J)$, is defined as:

$$
\chi(J) = \lim_{\Delta J \to 0} \frac{2[1 - F(J, \Delta J)^2]}{\Delta J^2} = \sum_{n \neq 0} \frac{|\langle \Psi_n(J)|H|\Psi_0(J) \rangle|^2}{E_n(J) - E_0(J)^2},
$$

which does not depend on the value of $\delta J$. It is proved to be related to the correlation function [31] which is usually used to indicate phase transitions.

The numerical results of the fidelity susceptibility versus $J$ for $N = 10, 50, 110, 190$ are shown in figure 5(a). We can see that the fidelity susceptibility peaks at the quasi-critical point $J'_N$, while its value is close to zero away from the quasi-critical point. Similar to the discussion in the above subsection, the quasi-critical point $J'_N$ also depends on the particle number $N$. Meanwhile, we can find that the maximum value of the fidelity susceptibility becomes larger and the quasi-critical point $J'_N$ gets closer to $J_c$ as $N$ increases. In order to study the effect of the finite particle number $N$ on the critical behaviour, we show the finite-size scaling behaviours of $\Delta J' = J'_N - J_c$ and $(\chi_{\text{max}})^{-1}$ for different $U$ with power-law expressions $\Delta J' \propto N^{-\delta_{\nu}}$ and $(\chi_{\text{max}})^{-1} \propto (N^\nu)^{-1}$ in figures 5(b) and (c), where the scaling exponents of $\Delta J'$ and $\chi_{\text{max}}$ are $\delta_{\nu} = 2/3$ and $\nu = 1.305$, respectively. We can find clearly that both $\Delta J'$ and $(\chi_{\text{max}})^{-1}$ converge to zero for $U = 0, 2, 4, 6, 8$ with different slopes when $N^{-\delta_{\nu}}$ and $(N^\nu)^{-1}$ approach zero, respectively. In other words, $J'_N$ approaches $J_c$ and $\chi_{\text{max}}$ diverges in the thermodynamic limit. So as to observe the quantum phase transition, we check the scaling behaviours for different values of $U$. For example, the finite-size scaling analysis of the fidelity susceptibility with $U = 2 g$ for different system sizes is shown in figure 5(d). According to the finite-size scaling ansatz and the power-law divergence shown in figure 5(c), the rescaled fidelity susceptibility around the critical point takes the form $\chi(\frac{J-J_c}{\xi}) = f_\nu([N^\nu(J-J_c)])$ with the correlation length $\xi \propto N^{-\nu}$, where $\nu = 2/3$. The scaling function $f_\nu(x)$ should be universal for large $N$ in this quantum phase transition. As shown in figure 5(d), all the data of different system sizes $N = 130, 150, 170, 190, 210$ collapse onto a single curve. It implies that the system at the critical point is scaling invariant with $\nu = 2/3$.

### 3.3. Entanglement entropy

If the system can be viewed as a bipartite system, the entanglement entropy of its ground state, which measures quantum correlations between partitions, is physically meaningful and has been used to characterize the quantum
phase transition [9, 11, 13, 27, 32, 33]. The von Neumann entropy, one typical entanglement entropy, of a bipartite system AB for a pure state $|\Psi\rangle$ is defined as

$$S = -\text{Tr}(\rho_A \log_2 \rho_A) = -\text{Tr}(\rho_B \log_2 \rho_B),$$

where $\rho_{AB} = \text{Tr}_{B(A)}(|\Psi\rangle\langle\Psi|)$ is the reduced density matrix of the system with two subsystems A and B. In this work, we consider the two atomic modes as subsystem A and the molecular mode as subsystem B. From the Schmidt decomposition of pure state, we know that the entanglement entropies calculated from the reduced density operator of the subsystem A and B agree well with each other. Following the definition, we numerically calculate the entanglement entropy between the two subsystems for the exact ground state and show the results in the inset of figure 6(a) with different system sizes $N = 10, 50, 110, 190$. The overall up-shift of the entanglement entropy is observed as $N$ increases for large $J$, whereas, unlike the behaviour of the Lipkin–Meshkov–Glick model [23, 34, 35], the entanglement entropy of our system does not diverge logarithmically at the critical point. Even so, it is exciting to note that the sudden rise of the entanglement entropy takes place near the critical point. In order to describe the quantum phase transition, the first-order derivative of the entanglement entropy with respect to $J$ is introduced, and the numerical results are shown in figure 6(a). The maximum value $(dS/dJ)_{\text{max}}$ appears at the critical points $J'_{\text{c}}$ which gets closer to $J_c$ as $N$ increases. The larger the size sample $N$, the larger the value of peak $(dS/dJ)_{\text{max}}$. The position $J'_{\text{c}}$ of $(dS/dJ)_{\text{max}}$ gets closer to $J_c$ as the system size $N$ increases. So as to find the dependence of $\Delta J' = J'_{\text{c}} - J_c$ and $(dS/dJ)_{\text{max}}$ on the system size $N$, we show their scaling behaviours with $\Delta J' \propto N^{-b}$ and $[(dS/dJ)_{\text{max}}]^{-1} \propto (N^\omega)^{-1}$ for different $\bar{U}$ in figures 6(b) and (c), where the scaling exponents of $\Delta J'$ and $[(dS/dJ)_{\text{max}}]^{-1}$ are $b = 2/3$ and $\omega = 0.713$, respectively. We find that both $\Delta J'$ and $[(dS/dJ)_{\text{max}}]^{-1}$ converge to zero for various $\bar{U}$ with different slopes when $N' = \omega$ and $(N^\omega)^{-1}$ approach zero, so that $J'_{\text{c}}$ approaches $J_c$ and $(dS/dJ)_{\text{max}}$ diverges when the thermodynamic limit $N \to \infty$. In other words, the entanglement property of the system at the critical point changes suddenly. In order to further investigate the quantum phase transition, we check the scaling behaviour for different values of $\bar{U}$. Regarding $\bar{U} = 2g$ as an example, the finite-size scaling analysis of the first-order derivative of the entanglement entropy with respect to $J$ for different system sizes is shown in figure 6(d). The finite-size scaling ansatz takes the form $(dS/dJ)_{\text{max}} / (dS/dJ) - 1 = f_1(N' (J - J'_{\text{c}}))$ with the correlation length critical exponent $\nu = 2/3$. The scaling function $f_1(x)$ should be universal for large $N$ in this quantum phase transition. As shown in figure 6(d), all the data of different system sizes $N = 130, 150, 170, 190, 210$ collapse...
where the discrete points denote the numerical results for finite particle numbers.

Phase boundary to non-degenerate and the fidelity decreases suddenly at the critical point. We have found that the ground state changes from degenerate to non-degenerate and the energy gap between the first excited state and the ground one. We have studied the fidelity for the ground state and the energy gap varying the intensity of the laser. By solving the fixed points, we have shown that the quantum phase transition from a PM phase to a mixed AM phase happens at the critical point. We have further examined the quantum phase transition in the full quantum approximation (MFA), we have given the phase diagram for the ground state onto a single curve. It suggests that the system at the critical point is scaling invariant with $\nu = 2/3$.

**4. Summary**

In this paper, we have studied the phase transition in an atom–molecule (AM) conversion system where the atoms can transit between two atomic hyperfine states. In the mean-field approximation (MFA), we have given the phase diagram for the ground state, and shown that the phase boundary between the pure molecule (PM) phase and the mixed AM one depends only on the atomic transition strength $J$ and the energy detuning $\delta_b$, but not on the atomic interaction $\tilde{U}$. The energy detuning $\delta_b$ can be modulated by tuning the magnetic field or the frequency of the laser, while the modulation of the atomic transition strength $J$ can be achieved by a different experimental means: varying the intensity of the laser. By solving the fixed points, we have studied the fidelity for the ground state and the energy gap between the first excited state and the ground one. We have found that the ground state changes from degenerate to non-degenerate and the fidelity decreases suddenly at the phase boundary $J_c = -3\delta_b/4 - \sqrt{2}g/2$, which implies that the energy gap and the fidelity may be characterized by the phase transition in the MFA.

In comparison to the mean-field results, we have investigated the quantum phase transition in the full quantum method. Taking the total population of atoms as the order parameter, we have shown that the quantum phase transition from a PM phase to a mixed AM phase happens at the critical point. We have further examined the quantum phase transition by calculating the energy gap between the first excited and the ground states, the fidelity susceptibility of the exact ground state, and the entanglement entropy between the atomic subsystem and molecular subsystem and its first-order derivative with respect to the transition strength $J$. The finite-size scaling behaviours of the energy gap, the fidelity susceptibility and the first-order derivative of the entanglement entropy for the ground state with respect to $J$ have been estimated, which obey the power law, i.e., $\Delta E_{\text{min}} \propto N^{-\mu}$, $\chi_{\text{max}} \propto N^\nu$ and $(dS/dJ)_{\text{max}} \propto N^\omega$ with their scaling exponents $\mu = 1/3$, $\gamma = 1.305$ and $\omega = 0.713$, respectively. In the limit of $N \to \infty$, the energy gap minimum at the critical point is zero, which agrees well with the result in the MFA. The critical exponent $\mu$ of $\Delta E_{\text{min}}$ has been estimated in the limits of both large $N$ ($N \gg 1$) and strong interaction ($\tilde{U} \gg 1$). The phase boundary obtained by the full quantum means in the thermodynamic limit coincides with that in the MFA as expected. 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the entanglement entropy have been shown with the correlation length critical exponent $\nu = 2/3$, which is the same as that of the Lipkin–Meshkov–Glick model [23, 24]. The scaling behaviour of the fidelity susceptibility shows a power-law divergence around the critical point, which is similar to that of the Lipkin–Meshkov–Glick model. However, the finite-size scaling behaviour of the entanglement entropy, which is analogous to that of the interacting AM boson model [11], does not diverge logarithmically at the critical point. Our results enrich the phenomena of the quantum phase transition in multi-component systems, especially the AM conversion system, and indicate that one can control the quantum phase transition of the AM conversion system by varying the transition strength between the two atomic hyperfine states as well as the AM energy detuning.

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