

Quantum phase transition from mixed atom-molecule phase to pure molecule phase: Characteristic scaling laws and Berry-curvature signature

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We investigate the quantum phase transition in an ultracold atom-molecule conversion system. It is found that the system undergoes a phase transition from a mixed atom-molecule phase to a pure molecule phase when the energy bias exceeds a critical value. By constructing a coherent state as variational state, we get a good approximation of the quantum ground state of the system. Using this variational state, we deduce the critical point analytically. We then discuss the scaling laws characterizing the transition and obtain the corresponding critical exponents. Furthermore, the Berry curvature signature of the transition is studied. In particular, we find that the derivatives of the Berry curvature with respect to total particle number intersect at the critical point. The underlying mechanism of this finding is discussed as well.

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I. INTRODUCTION

The quantum phase transition (QPT) describes a fundamental change in the properties of the ground state of a many-body system [1,2] and originates from the singularity of the energy spectrum [3]. It is of great interest and has seen a significant development from both the theoretical and experimental sides in a number of systems such as quantum Hall systems, fractional quantum Hall liquids, and quantum magnets [1]. In contrast with others, the cold atom systems are of special interest and have opened up a new route to investigate the QPT due to the advantages of the intrinsic cleanliness and the remarkable controllability of the physical parameters.

Experimental observation of the QPT from a superfluid (SF) to a Mott insulator (MI) in the ultracold atomic systems [4] has stimulated more extensive theoretical and experimental researches into this field [5,6]. The Bose-Hubbard model (BHM) [7], as a theoretical model which embodies the essential features of the above bosonic systems, plays an important role in studying the SF-MI phase transition [8,9]. In addition, the coupled atom-molecule boson model [10–12] currently attracts much theoretical attention for its application in the creation of ultracold molecules in experiments via Feshbach resonance (FR) [13–15] or photoassociation (PS) [16–18]. The QPT in the bosonic atom-molecule system has been addressed from the perspective of von Neumann entanglement entropy and fidelity [19], in contrast to the well-known BCS-BEC crossover phenomena in the fermionic systems [20,21]. Nevertheless, the critical behaviors and scaling laws associated with the QPT in such a bosonic atom-molecule conversion system keep unknown and call for further investigation.

In the present paper, we focus on the critical behaviors and scaling laws associated with the phase transition from an atom-molecule mixture phase to a pure molecule phase. With the help of coherent-state (CS) description, we can deduce the explicit expression of the critical point analytically. We

then discuss the scaling laws and obtain the critical exponents analytically or numerically. The Berry curvature signature associated with the phase transition is discussed as well.

The rest of the paper is organized as follows. Section II gives the many-body coupled atom-molecule model and the CS description. In Sec. III, we discuss the QPT in the system and show its Berry curvature signatures. Section IV presents our conclusion.

II. MANY-BODY MODEL AND COHERENT-STATE DESCRIPTION

We adopt the following two-channel second-quantized Hamiltonian to describe our bosonic atom-molecule conversion system [22]:

$$\hat{H} = -\frac{\gamma}{2}(\hat{a}^\dagger\hat{a} - \hat{b}^\dagger\hat{b}) + \frac{c_a}{V}(\hat{a}^\dagger\hat{a})^2 + \frac{c_b}{V}(\hat{b}^\dagger\hat{b})^2 + \frac{c_{ab}}{V}\hat{a}^\dagger\hat{a}\hat{b}^\dagger\hat{b} + \frac{g}{2\sqrt{V}}(\hat{a}^\dagger\hat{a}^\dagger\hat{b} + \hat{b}^\dagger\hat{a}\hat{a}), \quad (1)$$

where \hat{a} and \hat{b} are annihilation operators for atomic mode and molecular mode, respectively. The parameter γ denotes the energy difference between two modes while the parameter g characterizes the atom-molecule coupling strength. The parameter c_j describes s -wave scattering, taking into account the atom-atom (c_a), molecule-molecule (c_b), and atom-molecule (c_{ab}) interactions. The Hamiltonian commutes with the total atom number $N = \hat{a}^\dagger\hat{a} + 2\hat{b}^\dagger\hat{b}$ and $n = N/V$ is the particle density with V being the quantum volume.

For convenience, hereafter we assume that N is an even number and thus $M = N/2$ denotes the maximum number of the atomic pairs. Here we first introduce an atom-pair creation operator by

$$(\hat{c}^\dagger)^m \equiv \sqrt{\frac{m!}{(2m)!}}(\hat{a}^\dagger)^{2m}. \quad (2)$$

Each atomic pair is restricted to occupy a Hilbert space spanned by two orthonormal eigenvectors $|1\rangle$ and $|2\rangle$, and we denote

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the corresponding single-particle creation operators by \hat{c}^\dagger and \hat{b}^\dagger . Thus the Hilbert space of the N particle system reduces to be $M + 1$ dimensional and spanned by the eigenvectors in the Fock basis,

$$|m, M - m\rangle = [m!(M - m)!]^{-1/2}(\hat{c}^\dagger)^m(\hat{b}^\dagger)^{M-m}|0\rangle, \quad (3)$$

or $|2m, M - m\rangle = [(2m)!(M - m)!]^{-1/2}(\hat{a}^\dagger)^{2m}(\hat{b}^\dagger)^{M-2m}|0\rangle$, where m is the half population of particles in atomic mode \hat{a} and $|0\rangle$ is the vacuum state. In the above Fock-state representation, we construct the coherent states (i.e., Gross-Pitaevskii states) [23] as follows:

$$|\Psi_{\text{CS}}\rangle = \frac{1}{\sqrt{M!}}[\alpha\hat{c}^\dagger + \beta\hat{b}^\dagger]^M|0\rangle, \quad (4)$$

where α and β are complex amplitudes which satisfy the normalized condition $|\alpha|^2 + |\beta|^2 = 1$. The above coherent state (4) can be expressed as $|\Psi_{\text{CS}}\rangle = \sum_{m=0}^M \sqrt{\frac{M!}{m!(M-m)!}} \alpha^m \beta^{M-m} |2m, M - m\rangle$. According to the variational principle, by computing the expectation value $\langle\Psi_{\text{CS}}|\hat{H}|\Psi_{\text{CS}}\rangle$ and minimizing it, one can determine the values of α and β for the ground state of the system. On the other hand, in terms of the Fock states the Hamiltonian (1) becomes an $(M + 1) \times (M + 1)$ matrix, and then the ground state $|\Psi_{\text{GS}}\rangle = \sum_m C_m |2m, M - m\rangle$ can be found by directly diagonalizing the Hamiltonian matrix numerically. We have compared our coherent states with the quantum ground states of the second-quantized model (1), and the results are demonstrated in Fig. 1. For varied particle interactions, the good agreement has been seen. Actually, the coherent state (4) gives a well approximation of the quantum ground state in the large particle number limit [24].

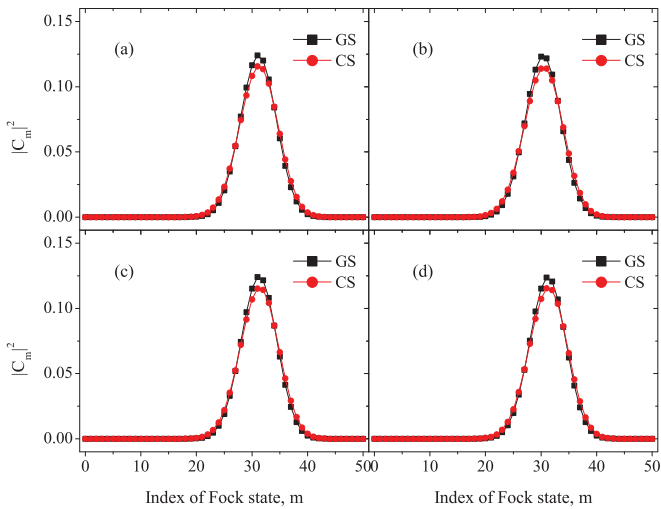


FIG. 1. (Color online) The comparison between the quantum ground states (GS) and our coherent states (CS) for different cases: (a) $c_a = c_b = c_{ab} = 0$; (b) $c_a = 0.02, c_b = c_{ab} = 0$; (c) $c_a = c_{ab} = 0, c_b = 0.02$; (d) $c_a = c_b = 0, c_{ab} = 0.02$. The parameters are $\gamma = -0.1, g = n = 1$, and $N = 100$.

III. QUANTUM PHASE TRANSITION

A. Characteristic scaling laws

The above two-channel model (1) brings a good opportunity to study the QPT in an ultracold atom-molecule conversion system. The coupling terms of atoms and diatomic molecules (i.e., $\hat{a}^\dagger\hat{a}^\dagger\hat{b} + \text{H.c.}$) bring a new gauge structure to the system [25], and thus we expect that they lead to some novel critical properties of the many-body system. In the following study we only focus our attention on the situation that the particle interactions are absent. For this case the analytical solution can be obtained. We first calculate the ground states of the system for the infinite particle number case. With the help of the variational state (4), the expectation value of \hat{H} is given by

$$\begin{aligned} \mathcal{H} &= \lim_{N \rightarrow \infty} \frac{\langle\Psi_{\text{CS}}|\hat{H}|\Psi_{\text{CS}}\rangle}{M} \\ &= -\frac{\gamma}{2}(2|\alpha|^2 - |\beta|^2) + \frac{g\sqrt{2n}}{2}(\alpha^*\alpha^*\beta + \beta^*\alpha\alpha), \end{aligned} \quad (5)$$

where α^* (β^*) is the conjugate complex of the parameter α (β). For convenience, we express the above two variables as $\alpha = |\alpha|e^{i\theta_\alpha}$ and $\beta = |\beta|e^{i\theta_\beta}$. Considering the conserved condition $|\alpha|^2 + |\beta|^2 = 1$, we introduce two new variables $s = |\beta|^2$ and $\theta = \theta_\beta - 2\theta_\alpha$. Using these new notations, we obtain (up to a trivial constant)

$$\mathcal{H}(s, \theta) = \frac{3}{2}\gamma s + g\sqrt{2n}(1-s)\sqrt{s} \cos \theta. \quad (6)$$

According to the variational principle, we minimize the energy $\mathcal{H}(s, \theta)$ with s and θ as variational parameters. We then obtain the optimum values [i.e., $(\bar{s}, \bar{\theta})$] of parameters for the ground state as follows:

$$(\bar{s}, \bar{\theta}) = \begin{cases} (1, \bar{\theta}), & \gamma < \gamma_c, \\ \left(\frac{4g^2n + 3\gamma^2 - \gamma\sqrt{24g^2n + 9\gamma^2}}{12g^2n}, \pi \right), & \gamma > \gamma_c, \end{cases} \quad (7)$$

where $\gamma_c = -g\sqrt{8n/9}$ is the critical point associated with the QPT of the system. When $\gamma > \gamma_c$ the system is in a mixed atom-molecule phase and when $\gamma < \gamma_c$ the system is in a pure molecule phase. For the pure molecule phase, $\bar{s} = 1$ thus the relative phase $\bar{\theta}$ cannot be defined.

Now we discuss the critical properties of the ground state. Indeed, above the threshold (i.e., $\gamma > \gamma_c$), the molecular fraction in the ground state \bar{s} can be expanded as follows:

$$\bar{s} = \frac{2\gamma^2 + 3\gamma_c^2 - 2\gamma\sqrt{\gamma^2 + 3\gamma_c^2}}{9\gamma_c^2}, \quad (8)$$

and the scaling behavior of the quantity \bar{s} for our system in the vicinity of the critical point is then found to be

$$\bar{s}(\gamma \rightarrow \gamma_c) = 1 + \frac{\gamma - \gamma_c}{\gamma_c}. \quad (9)$$

From this equation, we see that the corresponding critical exponent is one. It is to be mentioned that the particle interactions do not change the above scaling behavior but only change the value of the critical point. This is because, in the presence of particle interactions, the critical point becomes $\gamma_c = -\sqrt{8n/9}g + 2n(c_{ab} + c_b)/3$ and the scaling behavior of \bar{s} near the critical point takes the form of $\bar{s}(\gamma \rightarrow \gamma_c) = f_0 + f_1(\gamma - \gamma_c)$ (the explicit expressions are

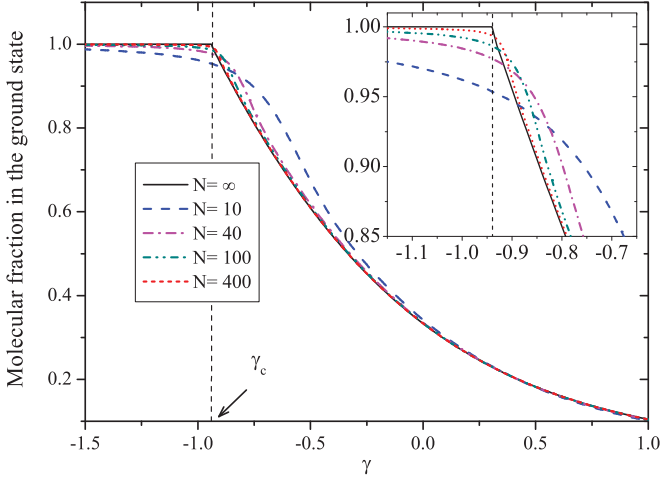


FIG. 2. (Color online) The molecular fraction in the ground state as a function of parameter γ (in units of $g\sqrt{n}$). Inset gives the partly enlarged image.

generally too messy to be shown here), where f_0 and f_1 are two constants which are determined by the coupling and interaction parameters. Obviously, the corresponding critical exponent is still one.

To gain more information associated with the quantum phase transition in the system, we have to study the ground states of the system and their properties in the finite particle number cases. By diagonalizing the Hamiltonian matrix numerically, we have obtained the ground states with different total particle numbers. The results are shown in Fig. 2. From Fig. 2, we see that the molecular fraction in the ground state (i.e., $\sum_m |C_m|^2 \frac{M-m}{M}$) increases as the ratio of the energy difference between two modes to the coupling strength between two modes decreases.

To get insight into the quantum phase transition in the system, we need to analyze the energy gap between the first excited state and the ground state. We have numerically calculated the energy levels of the second-quantized model (1) with different particle numbers. The results show that the dimensionless energy gap Δ between the ground state and the first excited state has a minimum near the critical point $\gamma_c = -g\sqrt{8n/9}$. To study the scaling behavior of the energy gap near the critical point, we denote the position of the minimum gap by γ_N , which is a function of particle number N . We find that as N increases the energy gap decreases and γ_N approaches the value γ_c . The point γ_N can be regarded as a pseudocritical point of the N -particle system. We particularly evaluate the minimum value of the energy gap Δ for different N , and the scaling behavior of the energy gap at the critical point is found to be [see Fig. 3(c)]

$$\Delta_{\min}(N) \simeq \mathcal{J}(\gamma_N - \gamma_c)^{z\nu}, \quad (10)$$

where $\mathcal{J} = 0.405$ is a constant, and $z\nu = 3/2$ denotes the critical exponents. The value of $z\nu$ is usually universal, that is, it is independent of most of the microscopic details of the Hamiltonian $\hat{H}(\gamma)$. For our system, we can regard the particle number N as the correlation length scale and estimate

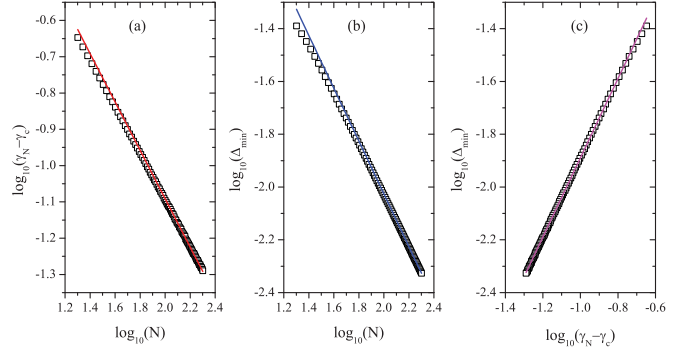


FIG. 3. (Color online) (a) The offset between γ_N and γ_c versus the total particle number N . (b) The minimum value of the energy gap Δ_{\min} at the pseudocritical point γ_N versus the total particle number N . (c) The minimum value of the energy gap Δ at the pseudocritical point versus the offset between γ_N and γ_c . Solid lines are plotted for guiding eyes, respectively, (from left to right) with the slopes being $-2/3$, -1 , and $3/2$.

the relation between this length scale and the pseudocritical point γ_N .

$$\Delta(\gamma_N - \gamma_c)^\nu \simeq N^{-1}, \quad (11)$$

where $\nu = 3/2$ is a critical exponent and $\Lambda \simeq 0.4335$ is a constant. The pseudocritical point changes and tends as $N^{-2/3}$ toward the critical point and clearly approaches γ_c as $N \rightarrow \infty$ [see Fig. 3(a)]. The ratio of Eqs. (10) and (11) gives the exponent z , which can be regarded as the dynamic critical exponent.

$$\Delta_{\min}(N) \simeq \Gamma N^{-z}, \quad (12)$$

where $\Gamma \simeq 0.9427$ and $z = 1$. This exponent is equal to the exponent obtained in Eq. (9) for the infinite particle number case. For our system, it is noted that the minimum energy separation between the ground and the first excited states decreases quite rapidly as the thermodynamical limit is approached. In fact, the minimum gaps Δ_{\min} scale, typically as N^{-1} , tend to zero when $N \rightarrow \infty$ [see Fig. 3(b)].

B. Berry curvature signature

The above analysis has confirmed that for our system the process from atom-molecule mixture to pure molecule is a quantum phase transition. In a general case, the quantum phase transition can occur at level crossings or avoided level crossings, and these kinds of level structures usually can be captured by the geometric phase of the ground state [26]. In this subsection, we will explore the connection between this quantum phase transition and the Berry curvature. To investigate the Berry phase, one needs to rewrite the coupling term in model (1) by introducing a parameter ϕ as follows [27]:

$$\frac{g}{2\sqrt{V}}(e^{i\phi}\hat{a}^\dagger\hat{a}^\dagger\hat{b} + e^{-i\phi}\hat{b}^\dagger\hat{a}\hat{a}). \quad (13)$$

In order to calculate the Berry connection of the system, for simplicity, we fix the parameters γ and $g\sqrt{n}$, and only change the parameter ϕ adiabatically from 0 to 2π . We introduce the dimensionless adiabatic parameter of $v \sim |\frac{d\phi}{dt}| \sim \frac{1}{T}$ (T is the time duration) as the measure of how slow the parameter changes. The adiabatic parameter tends

to zero (i.e., $v \rightarrow 0$), which indicates the adiabatic limit. The quantum adiabatic theorem states that, if the quantum system is initially prepared in an eigenstate $|\Psi_n(\mathbf{R}(0))\rangle$ with $\mathbf{R}(t) = (\gamma, g\sqrt{n}e^{\pm i\phi(t)})$, at time $t = T$, the system will be found in the eigenstate $|\Psi_n(\mathbf{R}(0))\rangle$ and a geometric phase factor will be acquired during the adiabatic process. This phase factor is independent of the time duration T and only related to the geometric property of the closed path in parameter space. At any instant, the eigenstates $|\Psi_n(\mathbf{R})\rangle$ of $\hat{H}(\mathbf{R})$ satisfy the eigenequation $\hat{H}(\mathbf{R})|\Psi_n(\mathbf{R})\rangle = E_n(\mathbf{R})|\Psi_n(\mathbf{R})\rangle$ with energy $E_n(\mathbf{R})$ ($n = 1, 2, 3, \dots$). Berry showed that the geometric phase for a specific eigenstate, such as the ground state $|\Psi_{\text{GS}}\rangle$ of the system we consider here, is given by [28]

$$\gamma_{\text{GS}}(C) = - \iint_C d\mathbf{S} \cdot \mathbf{B}(\mathbf{R}), \quad (14)$$

where C denotes an adiabatic closed path in parameter space and $d\mathbf{S}$ denotes the area element in parameter space. $\mathbf{B}(\mathbf{R})$ is the Berry curvature which takes the form of

$$\mathbf{B}(\mathbf{R}) \equiv \text{Im} \sum_{m \neq \text{GS}} \frac{\langle \Psi_{\text{GS}} | \nabla_{\mathbf{R}} \hat{H} | \Psi_m \rangle \langle \Psi_m | \nabla_{\mathbf{R}} \hat{H} | \Psi_{\text{GS}} \rangle}{(E_m - E_{\text{GS}})^2}. \quad (15)$$

The energy denominators in Eq. (15) show that the Berry curvature usually diverges at the point in parameter space where energy levels are cross and may have maximum values at avoided level crossings. Thus level crossings or avoided level crossings, the two specific level structures related to quantum phase transitions, are reflected in the geometry of the Hilbert space of the system and can be captured by the geometric phase of the ground state. For our avoided level crossings system (1), we plot the contour lines of the Berry curvature $|\mathbf{B}|$ for the ground state with different particle numbers in Fig. 4. The first and second particle number derivatives of Berry curvatures as a function of γ are also plotted in Fig. 5. From Fig. 5, we find that the lines (i.e., the first derivative of the Berry curvature) with different particle numbers cross at the point $\gamma_c = -g\sqrt{8n/9}$ which is the QPT point between the mixture phase and the pure molecule phase. Moreover, the second derivative of the Berry curvature reaches zero exactly at this point. This phenomenon is similar to the behavior of the entanglement as a function of system parameter for different system sizes [19]. This result is independent of system size, which implies that, even though a QPT is only rigorously defined in the thermodynamic limit $N \rightarrow \infty$, the Berry curvatures do exactly mark the changes in the ground states of the system for a finite particle number. In our system, the Berry curvature usually depends linearly on the

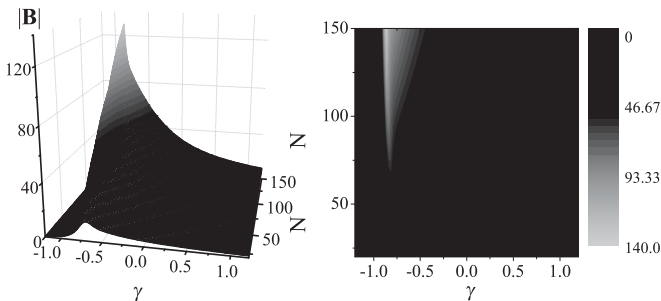


FIG. 4. Berry curvature $|\mathbf{B}|$ (left) and its contour map (right) for the ground state. The parameter γ is in units of $g\sqrt{n}$.

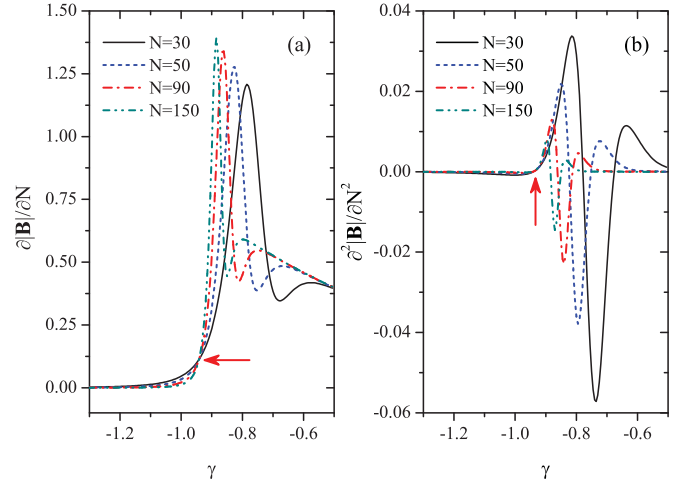


FIG. 5. (Color online) The first (left column) and second (right column) particle number derivatives of Berry curvature $|\mathbf{B}|$ for the ground state versus the dimensionless parameter γ (in units of $g\sqrt{n}$) with different N . The arrows denote the points of intersection.

particle number N [see Eq. (15) and Fig. 4], that is, $|\mathbf{B}| \propto N$ in the critical region. This is because the minimum energy gaps between the first excited state and the ground state converge to zero in the power law of $\frac{1}{N}$ [see Fig. 3(b) and Eq. (12)]. Then the first derivative of Berry curvature is an intensive quantity in the finite particle number limit. Similar to other approaches describing phase transitions, we can also extract critical points from the Berry curvature.

IV. CONCLUSION

In this work, we have constructed the coherent states for the ultracold atom-diatom molecule conversion system, which are found to be a nice approximation of the quantum ground states of the system in the large particle number limit. Based on the coherent states and using the variational method, we have discussed the quantum phase transition of the system and have obtained the critical point analytically. We find that the system exhibits a phase transition from an atom-molecule mixture phase to a pure molecule phase when the energy bias exceeds a critical value. Moreover, we have studied the scaling behaviors of the energy gap between the ground and the first excited states in the vicinity of the critical point. The characteristic scaling laws and the corresponding critical exponents have been derived analytically or numerically. The Berry curvature signature of the transition is discussed. In particular, we find that the derivatives of the Berry curvature with respect to total particle number intersect at the critical point. The underlying mechanism of this finding is discussed as well.

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