Static Gross-Pitaevskii equations for the molecular achiral-chiral transitions

Chong Ye, Quansheng Zhang, Yong Li

1 Beijing Computational Science Research Center, Beijing 100193, China
2 Synergetic Innovation Center for Quantum Effects and Applications, Hunan Normal University, Changsha 410081, China

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I. INTRODUCTION

The stabilization of chiral molecules either in a left-handed $|L\rangle$ or as the right-handed mirror image $|R\rangle$ is an old but important problem in molecular quantum mechanics. According to the quantum theory, the molecules might be expected in the ground state of the parity-invariant molecular Hamiltonian, corresponding to the symmetric superposition of these chiral states. It is explained with the exceedingly long tunneling time [1] between $|L\rangle$ and $|R\rangle$ as well as introducing party-violating terms [2–7] in the molecular Hamiltonian. These mechanisms considering the Hamiltonian of an isolated molecule are hardly sufficient to explain the observed stabilization of many chiral molecules.

In fact, isolated molecules do not exist in nature. The effects of the environment must be taken into consideration. The intermolecular interaction is one of the effects of the environment attributing to the stabilization of chiral molecules [8–12]. Many approaches have been proposed to quantitatively deal with the effect of the intermolecular interaction, where the most well-known ones are the mean-field theory [13–15] and the decoherence theory [16–22]. There are also proposals combining the mean-field and the decoherence theories to study the stabilization of chiral molecules [23, 24]. In the mean-field theory, the stabilization of chiral molecules is the result of a quantum phase transition from an achiral phase to a chiral phase [14, 15], namely the achiral-chiral transition. In the decoherence theory, the stabilization of chiral molecules can be understood [16] in analogy to the quantum Zeno effect [25] when the environment is treated as continuously monitoring the molecular state.

Using the mean-field theory, Jona-Lasinio and coworkers [14, 15] introduced a very simple model in the vibrational dimension to explore the static and evolution problems of chiral molecules. It quantitatively describes, without free parameters, the effect of the intermolecular interaction when the gas molecules of the same type are interacting via electric dipole-dipole interactions. This approach explains the stabilization of chiral (or polar) molecules whose electric dipoles change in sign for $|L\rangle$ and $|R\rangle$ (e.g., $D_2S_2$, $NH_3$, and $ND_3$). However, for many chiral molecules which do not admit such a property (e.g., $1,2$–propanediol, 1,3–butanediol, and carvone), this procedure [14, 15] is not available [23]. Vardi [13] introduced a mean-field model in the vibrational dimension available for all chiral molecules. In the model [13], the difference between homochiral and heterochiral interactions [26, 27] is considered attributing to the stabilization of chiral molecules. However, such a difference due to involving both the electric and magnetic dipoles [28–30] may be too slightly. In addition, the model [13] has free parameters.

In this paper, we consider the effect of the intermolecular interaction when the gas molecules of the same type are interacting via electric dipole-dipole interactions. In the vibrational dimension, we assume each molecule is in the same state. Since the system is translationally and rotationally invariant, we introduce the two-particle density of the thermal equilibrium state in the spatial and rotational dimensions [31]. It can be approximately expressed [31] in the form of a power exponent function of electric dipole-dipole interactions varying with the state in the vibrational dimension. With these, we give static Gross-Pitaevskii (G-P) equations in the vibrational dimension from the many-body Hamiltonian of the molecular gases via the method of Lagrange multipliers. Our G-P equations have no free parameters and can be applied to all chiral molecules. Exploring chiral molecules with our static G-P equations, we find that the achiral-chiral transitions can be classified into two categories. While in one category the mean-field ground state changes con-
continuously from the achiral ground state of the parity-
invariant molecular Hamiltonian to one of two degener-
ated chiral states with the increase of the intermolecular
interaction, in the other category the mean-filed ground
state changes discontinuously. In order to summarize
our results, we give the mean-field phase diagram of the
achiral-chiral transitions. We also study the nonpolar-
nonpolar transitions of polar molecules and compare our re-
results for NH$_3$ (ND$_3$) molecules with those predicted with
the model in Refs. [14, 15].

II. MODEL

A. Many-body Hamiltonian

Without taken the kinetic and rotational energies of single
molecules into consideration [13–16, 18, 20, 22, 23], the many-body Hamiltonian for the system of $N$
molecules is

$$\hat{H} = \sum_{i=1}^{N} \left( -\frac{\tilde{\omega}}{2} |L\rangle_{ii} \langle R| + h.c. \right) + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \hat{V}(r_{ij}^{e}, \mu^{s,i}, \mu^{s,j}),$$

where the first term is the parity-invariant molecular
Hamiltonian in the basis \{\{L\}, \{R\}\} and the second term
is the standard electric dipole-dipole interaction between
the $i$th and $j$th molecules located at $r_{ij}^{e}$ and $r_{ij}^{e}$. It can
be written as

$$\hat{V}(r_{ij}^{e}, \mu^{s,i}, \mu^{s,j}) = \frac{\mu^{s,i} \cdot \mu^{s,j} - 3(\mu^{s,i} \cdot r_{ij}^{e})(\mu^{s,j} \cdot r_{ij}^{e})r_{ij}^{-2}}{4\pi \varepsilon_0 r_{ij}^3}.$$  \hfill (2)

Here $\mu^{s,i}$ is the electric dipole operator of the $i$th
molecule in the space-fixed frame, the notation “$s$” indi-
cates the space-fixed frame, $r_{ij}^{e} = r_{ij}^{e} - r_{ij}^{e}$, and $r_{ij} = |r_{ij}^{e}|$. We have

$$r_{ij}^{s} = r_{ij} \sum_{\sigma = 0, \pm 1} \sqrt{\frac{4\pi}{3}} Y_{1\sigma}(\alpha_{r_{ij}}, \beta_{r_{ij}}, \gamma_{r_{ij}}) e_{r_{ij}}^s,$$  \hfill (3)

where $\Omega_{r_{ij}} = (\alpha_{r_{ij}}, \beta_{r_{ij}}, \gamma_{r_{ij}})$ are the solid angles of $r$s and
$Y_{1\sigma}(...) = Y_{1\sigma}(\alpha_{r_{ij}}, \beta_{r_{ij}}, \gamma_{r_{ij}})$ are the spherical harmonics. Here $e_{r_{ij}} = e_z$ and
$e_{r_{ij}} = (e_x - ie_y)/\sqrt{2}$ with the coordinations in
the space-fixed frame $(X, Y, Z)$. The components of the electric
dipole operator in the space-fixed frame can be obtained
by a rotation from the molecular frame [32]

$$\mu^{s}_{\sigma} = \sum_{\sigma' = 0, \pm 1} \left[ D^1_{\sigma\sigma'}(\alpha, \beta, \gamma) \right]^{*} \mu^{m}_{\sigma'},$$  \hfill (4)

with $\mu^{\pm}_{\sigma} = \mu^{\pm}_{x}$ and $\mu^{\pm}_{\sigma'} = (\mp \mu^{x}_{\sigma'} - i\mu^{y}_{\sigma'})/\sqrt{2}$. The index “$m$” indicates the molecular frame and “$s$” denotes taking conjugate complex. $D^1$ is the rotation matrix in three dimensions. Here $\Omega = (\alpha, \beta, \gamma)$ are the Euler angles denoting the orientation of the molecule.

B. Static Gross-Pitaevskii equations in the vibrational dimension

We assume the many-body state of an $N$-molecule sys-
tem is

$$\{|\Psi\rangle = \left( \prod_{i=1}^{N} \otimes |\lambda\rangle_i \otimes |\psi_{sr}\rangle, \right) \hfill (5)$$

where “$sr$” denotes the spatial and rotational dimensions.
The wavefunction of $|\psi_{sr}\rangle$ is $\psi_{sr}(r_1^{e}, ..., r_N^{e}; \Omega_1, ..., \Omega_N)$. Each molecule is assumed in the vibrational state

$$|\lambda\rangle = |\varphi_{\lambda,L}\rangle |L\rangle + |\varphi_{\lambda,R}\rangle |R\rangle,$$  \hfill (6)

with $|\varphi_{\lambda,L}|^2 + |\varphi_{\lambda,R}|^2 = 1$.

The energy of the system, $E(|\Psi\rangle) = \langle \Psi | \hat{H} | \Psi \rangle$, is

$$E(|\Psi\rangle) = -\frac{N\tilde{\omega}}{2} (\varphi_{\lambda,L} \varphi_{\lambda,R} + h.c.) + \frac{N(N-1)}{2} g(\lambda)$$  \hfill (7)

with the two-particle interacting energy

$$g(\lambda) = \langle \psi_{sr} | V(r_{ij}^{e}, \mu^{s,i}, \mu^{s,j}) | \psi_{sr} \rangle.$$  \hfill (8)

Here $\mu^s_{\lambda} = \langle \lambda | \mu^s | \lambda \rangle$ and $V(...) = \frac{i}{\sqrt{2}} \langle \lambda \lambda | \hat{V}(...) | \lambda \lambda \rangle$ are operators in the spatial and rotational dimensions. Explicitly, we have $\langle \mu^s_{\lambda} \sigma \rangle = \langle \lambda | \mu^s | \lambda \rangle$.

$$V(r_{ij}^{e}, \mu^{s,i}, \mu^{s,j}) = -\frac{1}{4\pi \varepsilon_0 r_{ij}^3} \sum_{\sigma = 0, \pm 1} \mu^{m,i}_{\lambda,\sigma} \mu^{m,j}_{\lambda,\sigma} \times \\
\{ \sum_{\sigma' = 0, \pm 1} [D^1_{\sigma\sigma'}(\Omega_i) D^1_{\sigma'\sigma}(\Omega_j)] Y_{1\sigma}(\hat{\Omega}_{r_{ij}}) Y_{1\sigma'}(\hat{\Omega}_{r_{ij}}) \}.$$  \hfill (9)

In the molecular frame, the electric dipoles of the left-
and right-handed molecules are $\mu_{\lambda}^{m} = \langle \lambda | \mu^m | \lambda \rangle$ and $\mu_{R}^{m} = \langle R | \mu^m | R \rangle$. For chiral molecules, it is well
known [38–44]

$$\mu_{L,x}^{m} m_{L,y}^{m} m_{L,z}^{m} = -\mu_{R,x}^{m} m_{R,y}^{m} m_{R,z}^{m}.$$  \hfill (10)

We assume that the components obey

$$\mu_{L,x}^{m} = \mu_{R,x}^{m} = \mu^m_x,$ \hfill (11)$$

$$\mu_{L,y}^{m} = \mu_{R,y}^{m} = \mu^m_y,$ \hfill (11)$$

$$\mu_{L,z}^{m} = -\mu_{R,z}^{m} = \mu^m_z.$$  \hfill (11)

For the molecule in the state $|\lambda\rangle$, we have

$$\mu_{L,\pm 1}^{m} = \pm \mu^m_x - i \mu^m_y,$ \hfill (12)$$

$$\mu_{L,0}^{m} = \mu^m_z (|\varphi_{\lambda,L}|^2 - |\varphi_{\lambda,R}|^2).$$  \hfill (12)
In order to calculate \( g(\lambda) \), we introduce the two-particle density in the spatial and rotational dimensions \( \rho^\sigma_2(r_1^s, r_2^s; \Omega_1, \Omega_2) \). It is obtained from 

\[
|\psi_n(r_1^s, \ldots, r_N^s; \Omega_1, \ldots, \Omega_N)|^2
\]

by integrating all except two coordinates \((r_1, r_2)\) and two Euler angles \((\Omega_1, \Omega_2)\). Thus, we get 

\[
g(\lambda) = \int d^3r_1^s d^3r_2^s d\Omega_1 d\Omega_2 V(\ldots) \rho^\sigma_2(\ldots).
\]

The two-particle density can be approximately written as [31]

\[
\rho^\sigma_2(r_1, r_2; \Omega_1, \Omega_2) \simeq \frac{1}{Z} \exp\left[-\frac{V(r_{12}^s, \mu^{s,1}_1, \mu^{s,2}_\lambda)}{k_B T}\right]
\]

with the Boltzmann constant \( k_B \) and the normalization constant \( Z \). With Eq. (13), we assume the thermal equilibrium state in the spatial and rotational dimensions [31]. Since \( V(\ldots) \), and \( \rho^\sigma_2(\ldots) \) are functions of \( r_{12}^s \), we make variable substitution as 

\[
d^3r_1^s d^3r_2^s = d^3r_{12}^s d\Omega_1 d\Omega_2 V(\ldots) \rho^\sigma_2(\ldots) \]

and integrate over \( r_{12}^s \) first. We get 

\[
g(\lambda) = \frac{V}{k_B T} \int_{r_{12}^s > 0} r_{12}^{s,4} (4\pi\varepsilon_0 r_{12}^s)^2 24\pi (8\pi^2)^2 \frac{N}{\pi k_B T} \frac{\mu^{s,4}_\lambda}{(4\pi\varepsilon_0 k_B T)^2 d^3} \]

with the pressure of the gas \( P \), and the molecular collision diameter \( d \). We have used 

\[
\int d^3r_1^s d^3r_2^s d\Omega_1 d\Omega_2 V(\ldots) = 0, \quad Z \simeq (8\pi^2)^2 V^2, \quad PV = N k_B T.
\]

We note that 

\[
|\mu^{s,4}_\lambda/(4\pi\varepsilon_0 r_{12}^s)^2| \text{ is the Van der Waals potential between two electric dipoles, namely the Keesom interaction [36].}
\]

The average energy of a molecule \( \varepsilon(\lambda) \equiv E(\Psi)/N \) in the system with neglecting the terms of order \( 1/N \) is 

\[
\varepsilon(\lambda) = -\frac{\omega}{2} \langle \varphi_{\lambda,L} \varphi_{\lambda,R} + c.c. \rangle - \frac{4\pi}{9 \pi} \frac{P|\mu^{s,4}_\lambda|}{(4\pi\varepsilon_0 k_B T)^2 d^3}.
\]

Using the condition \(|\varphi_{\lambda,L}|^2 + |\varphi_{\lambda,R}|^2 = 1\), we can get the static Gross-Pitaevskii equations for the system in the vibrational dimension via the method of Lagrange multipliers as 

\[
-\frac{\omega}{2} \varphi_{\lambda,L} + U S_1^z(\lambda) \varphi_{\lambda,R} + G S_2(\lambda) \varphi_{\lambda,L} = \eta \varphi_{\lambda,L},
\]

\[
-\frac{\omega}{2} \varphi_{\lambda,R} - U S_1^z(\lambda) \varphi_{\lambda,L} - G S_2(\lambda) \varphi_{\lambda,L} = \eta \varphi_{\lambda,L},
\]

where the eigenvalue \( \eta \) is the chemical potential, 

\[
S_2(\lambda) \equiv |\varphi_{\lambda,L}|^2 - |\varphi_{\lambda,R}|^2,
\]

\[
U = \frac{(\mu^m_s)^4 P}{18\pi(\varepsilon_0 k_B T)^2 d^3},
\]

and 

\[
G = \frac{(\mu^m_s)^2 P}{18\pi(\varepsilon_0 k_B T)^2 d^3}
\]

with \( \mu^m_s = \sqrt{(\mu^m_s)^2 + (\mu^m_\lambda)^2} \).

It is worth to note that, in Refs. [13, 14], they mainly focused on the evolution problems. For the evolution problems, one can ignore the change of \( \rho^\sigma_2(\ldots) \) with time in the weak collision region, where any individual collision has but little effect on the orientation and spatial distribution of molecules [45]. With this, for chiral molecules, we can obtain the similar time-dependent G-P equations in the weak collision region as those in Refs. [13, 14] in the sense that the intermolecular interactions give rise to nonlinear terms proportional to \( S_2(\lambda) \). However, for static problems, the vibrational state dependence of \( \rho^\sigma_2(\ldots) \) should be taken into consideration and thus our static G-P equations (16) may give a more precise description.

### III. ACHIRAL-CHIRAL TRANSITION

Starting from the many-body Hamiltonian (1), we have obtained the static G-P equations for all the molecules with inversion symmetry in the vibrational dimension. In the following, we will explore the achiral-chiral transitions via solving the nonlinear eigenvalue problem associated with Eq. (16). The coefficients \( \varphi_{\lambda,L} \) and \( \varphi_{\lambda,R} \) can be chosen real. We find that they are the solutions of

\[
4 \varphi_{\lambda,L} \varphi_{\lambda,R} [U S_1^z(\lambda) + G S_2(\lambda)] = \omega S_2(\lambda).
\]

Once the solutions are found, the corresponding eigenvalues (chemical potential) are given by

\[
\eta = -\omega \varphi_{\lambda,L} \varphi_{\lambda,R} - U S_1^z(\lambda) - G S_2(\lambda).
\]

There are always two solutions of Eq. (20) such that \( S_2(\lambda) = 0 \) as shown in Fig. 1. Up to an irrelevant sign, they are 

\[
|\pm\rangle = \frac{1}{\sqrt{2}} (|L\rangle \pm |R\rangle)
\]

with corresponding eigenvalues \( \eta_{\pm} = \mp \omega/2 \). They are the ground and first excited eigenstates of the parity-invariant molecular Hamiltonian, respectively.

For a given \( G \equiv G/U \), there will be further chiral solutions to Eq. (20) when \( f \equiv \omega/U \) is smaller than a critical value \( f_{\text{cr}} \) as shown in Fig. 1. The corresponding chiral states have lower energies than the achiral state \(|+\rangle\). The decrease of \( f \) will give rise to the achiral-chiral transition. Changing \( G \), we find that the achiral-chiral transitions can be divided into two categories: in category (I) the mean-field ground state changes continuously from the achiral state \(|+\rangle\) to a chiral state with the decrease of \( f \), in category (II) the mean-field ground state changes discontinuously.

In Fig. 1 (a) and Fig. 1 (b), we choose \( G = 3 \) to show the typical behaviors of the achiral-chiral transitions in category (I). When \( f \) decreases from the region \( f > f_{\text{cr}} \) to the region \( f < f_{\text{cr}} \), the mean-field ground state will change continually from the achiral state \(|+\rangle\) to one of
Figure 1. Achiral-chiral transitions. (a) and (b) present the achiral-chiral transition in category (I) with \( \mathcal{G} = 3 \). (c) and (d) present the achiral-chiral transition in category (II) with \( \mathcal{G} = 0.4 \). Here \(|\pm\rangle\) are the two achiral states. Other states \(|\lambda_1\rangle, |\lambda_2\rangle, |\lambda_3\rangle\) and \(|\lambda_4\rangle\) are chiral in the sense \(|\lambda_1\rangle = \mathcal{T}|\lambda_2\rangle\) and \(|\lambda_3\rangle = \mathcal{T}|\lambda_4\rangle\) with the parity operator \( \mathcal{T} \).

the two degenerated chiral states \(|\lambda_1\rangle\) and \(|\lambda_2\rangle\). They are chiral in the sense [15] that \(|\lambda_1\rangle = \mathcal{T}|\lambda_2\rangle\) with the parity operator \( \mathcal{T} \). In the limit \( f \ll 1 \) \((\omega \ll U)\), we find that \(|\lambda_1\rangle\) and \(|\lambda_2\rangle\) approach the localized states \(|L\rangle\) and \(|R\rangle\), respectively. In category (II), the typical behaviors are shown in Fig. 1 (c) and Fig. 1 (d) with \( \mathcal{G} = 0.4 \). When \( f \) decreases from the region \( f > f_{cr} \) to the region \( f < f_{cr} \), the mean-field ground state jumps from the achiral state \(|\pm\rangle\) to one of the degenerated chiral states \(|\lambda_1\rangle\) and \(|\lambda_2\rangle\).

We find that there are further two chiral solutions \(|\lambda_3\rangle\) and \(|\lambda_4\rangle\) with \(|\lambda_3\rangle = \mathcal{T}|\lambda_4\rangle\) in the region \( f_{cr} < f < f_{cr}' \).

In Fig. 2, we show how \( f_{cr} \) and \( f_{cr}' \) vary with \( \mathcal{G} \). It can serve as the phase diagram in the \((\mathcal{G} - f)\) plane. The line of \( f_{cr}(\mathcal{G}) \) divides the plane into the upper and lower halves. The achiral states \(|\pm\rangle\) are always the mean-field eigenstates of the system with eigenvalues \( \eta_{\pm} = \mp \omega/2 \).

In the lower half plane, the system has two degenerated chiral eigenstates \(|\lambda_1\rangle\) and \(|\lambda_2\rangle\) with lower eigenvalues than \(|\pm\rangle\). In the area surrounded by \( f_{cr}(\mathcal{G}) \), \( f_{cr}(\mathcal{G}) \) and \( f\)-axis, there are further two degenerated chiral eigenstates \(|\lambda_3\rangle\) and \(|\lambda_4\rangle\) with lower eigenvalues than \(|\pm\rangle\). However \(|\lambda_3\rangle\) and \(|\lambda_4\rangle\) have higher eigenvalues than \(|\lambda_1\rangle\) and \(|\lambda_2\rangle\). The intersection of the lines of \( f_{cr}(\mathcal{G}) \) and \( f_{cr}'(\mathcal{G}) \) give the critical value \( \mathcal{G}_{cr} = 2 \) labeled with the vertical black dashed line. It divides the achiral-chiral transitions into categories (I) and (II). In category (I) where \( \mathcal{G} \geq \mathcal{G}_{cr} \), the mean-field ground state changes continuously from the achiral state \(|\pm\rangle\) to one of the two degenerated chiral states \(|\lambda_1\rangle\) and \(|\lambda_2\rangle\) with the decrease of \( f \). In category (II) where \( \mathcal{G} < \mathcal{G}_{cr} \), the mean-field ground state changes discontinuously.

Our results are different from those predicted with the models in Refs. [13–15]. With the model in Ref. [13], the achiral-chiral transitions are always continuous. In Refs. [14, 15], only \( \mathcal{G} = 0 \) is considered and they predicted a continuous phase transition. However, we find that when \( \mathcal{G} < \mathcal{G}_{cr} \) the achiral-chiral transitions are discontinuous.

IV. NONPOLAR-POLAR TRANSITION (\( \mathcal{G} = 0 \))

When \( \mathcal{G} = 0 \), the static G-P equations (16) can also be used to explore the nonpolar-polar transitions of polar molecules such as NH\(_3\) and ND\(_3\). In the following, we will give a comparison between the results of the nonpolar-polar transitions predicted by our static G-P equations and those in Refs. [14, 15].

The results are shown in Fig. 3. We predict a discontinuous phase transition from the nonpolar eigenstate \(|\pm\rangle\) to one of the two degenerated polar eigenstates \(|\lambda_1\rangle\) and \(|\lambda_2\rangle\), which is different from the continuous phase transition predicted by the model in Refs. [14, 15]. With our model, we predict other two degenerated polar eigenstates \(|\lambda_3\rangle\) and \(|\lambda_4\rangle\). The critical values of \( f \) predicted with our model and the model in Refs. [14, 15] are \( f_{cr}' = 0.7698 \) and \( f_{cr} = 1 \), respectively. Since \( \omega/U \propto P^{-1} \), the critical gas pressure is

\[
P_{cr} = \frac{18\pi\omega(\varepsilon_0k_BT)^2d^3}{(\mu m)^3f_{cr}} = \frac{9}{8\pi f_{cr}^2d^3}\frac{\omega}{T_z^2}.
\]

For the nonpolar-polar transition of NH\(_3\) (ND\(_3\)) at room
temperature of 300 K, the critical gas pressures predicted with our model and the model in Refs. [14, 15] are $P_{cr}^a = 2.251$ atm ($P_{cr}^a = 0.147$ atm) and $P_{cr}^b = 1.695$ atm ($P_{cr}^b = 0.111$ atm), respectively. The experimental value of the critical gas pressure is about 2.0 atm (0.131 atm) for NH$_3$.

\[ \lambda = 0 \]
\[ \lambda = 1 \]
\[ \lambda = 2 \]
\[ \lambda = 3 \]

\[ |\lambda| = 0 \]
\[ |\lambda| = 1 \]
\[ |\lambda| = 2 \]
\[ |\lambda| = 3 \]

Figure 3. Nonpolar-polar transition. (a) and (b) are results predicted by our model. (c) and (d) are results predicted by the model in Refs. [14, 15].

V. SUMMARY

Starting from the many-body Hamiltonian of the molecular gases with electric dipole-dipole interactions, we have given static G-P equations in the vibrational dimension to explore the achiral-chiral transitions as well as the nonpolar-polar transitions. For the achiral-chiral transitions, we have given the mean-field phase diagram in the $G - f$ plane. We find that, for $G > G_{cr}$, the mean-field ground state changes continuously from the achiral state $|+\rangle$ to one of the two degenerated chiral state $|\lambda_1\rangle$ and $|\lambda_2\rangle$ with the decrease of $f$, for $G < G_{cr}$ the mean-field ground state changes discontinuously. This is different from the results predicted with the models in Ref. [13–15], where the mean-field ground state always changes continuously. We have also studied the nonpolar-polar transition of polar molecules. Our model gives a discontinuous transition. The critical gas pressures for NH$_3$ and ND$_3$ molecules predicted by our model agree well with the experimental values.

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