Bose-Einstein condensates of microwave-shielded polar molecules

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Introduction

We investigate the ground-state properties of the ultracold gases of bosonic microwave-shielded polar molecules (MSPMs). To account for the large shielding core of the inter-molecular potential, we adopt a variational ansatz incorporating the Jastrow correlation factor. We show that the system is always stable and supports a self-bound gas (SBG) phase and an expanding gas (EG) phase. We also calculate the condensate fraction which is significantly reduced when the size of the shielding core of the two body potential becomes comparable to the inter-molecular distance. Our studies distinguish the molecular condensates from the atomic ones and invalidate the application of the Gross-Pitaevskii equation to the microwave-shielded molecular gases. Our work paves the way for studying the Bose-Einstein condensations of ultracold gases of microwave-shielded polar molecules.

Formulation

Model

We consider a gas of N interacting bosons at zero temperature

$$H = \int d\mathbf{r} \left[\frac{1}{2M}\nabla\hat{\psi}^\dagger(\mathbf{r})\nabla\hat{\psi}(\mathbf{r}) + V(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right] + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})$$

- The confining potential: $V(\mathbf{r}) = M[\omega_\perp^2(x^2+y^2)+\omega_z^2 z^2]/2$
- The effective potential for MSPMs: $U(\mathbf{r}) = C_3(3\cos^2\theta - 1)/r^3 + C_6\sin^2\theta(1+\cos^2\theta)/r^6$

Variational Ansatz and total energy

A variational wavefunction with Jastrow correlations (VWJC)

$$|\Psi\rangle = \frac{e^{-\alpha^2/2}}{\sqrt{\mathcal{N}}}\sum_N \frac{\alpha^N}{N!}\int D[\mathbf{r}]\prod_{i<j}^{N} J(\mathbf{r}_i,\mathbf{r}_j)\prod_{j=1}^{N}\phi_0(\mathbf{r}_j)\hat{\psi}^\dagger(\mathbf{r}_j)|0\rangle$$

- Normalized single-particle wavefunction: $\phi_0(\mathbf{r})$
- Jastrow correlation factor: $J(\mathbf{r}_i,\mathbf{r}_j)$ vanishes as $\mathbf{r}_i \to \mathbf{r}_j$ and approaches unit as $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$
- Density distribution: $n(\mathbf{r}) = \langle\Psi|\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})|\Psi\rangle$

To determine $J(\mathbf{r},\mathbf{r}')$ and the density amplitude $\phi(\mathbf{r}) = \sqrt{n(\mathbf{r})}$, we minimize the total energy

$$E = \int d\mathbf{r}\left[\frac{1}{2M}\nabla\phi(\mathbf{r})\nabla\phi(\mathbf{r}) + V(\mathbf{r})n(\mathbf{r})\right] + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' U_{\rm re}(\mathbf{r},\mathbf{r}')n(\mathbf{r})n(\mathbf{r}'),$$

where $U_{\rm re}(\mathbf{r},\mathbf{r}') = \{U(\mathbf{r}-\mathbf{r}')J^2(\mathbf{r},\mathbf{r}') + \frac{1}{M}[\nabla J(\mathbf{r},\mathbf{r}')]^2 + \frac{1}{4M}\nabla f(\mathbf{r},\mathbf{r}')\cdot\nabla\}\bar{g}_2(\mathbf{r},\mathbf{r}')$ is the two-body interaction renormalized by the hole excitations, $f(\mathbf{r},\mathbf{r}') = J^2(\mathbf{r},\mathbf{r}')-1$ and $\bar{g}_2(\mathbf{r},\mathbf{r}') = g_2(\mathbf{r},\mathbf{r}')/J^2(\mathbf{r},\mathbf{r}')$. In low and intermediate density regimes, we use the cluster expansion to calculate $\bar{g}_2(\mathbf{r},\mathbf{r}') = 1 + \int d\mathbf{r}_1 f(\mathbf{r},\mathbf{r}_1)n(\mathbf{r}_1)F(\mathbf{r}_1,\mathbf{r}')$ analytically, where $F(\mathbf{r},\mathbf{r}') = f(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}_1 f(\mathbf{r},\mathbf{r}_1)n(\mathbf{r}_1)F(\mathbf{r}_1,\mathbf{r}')$.

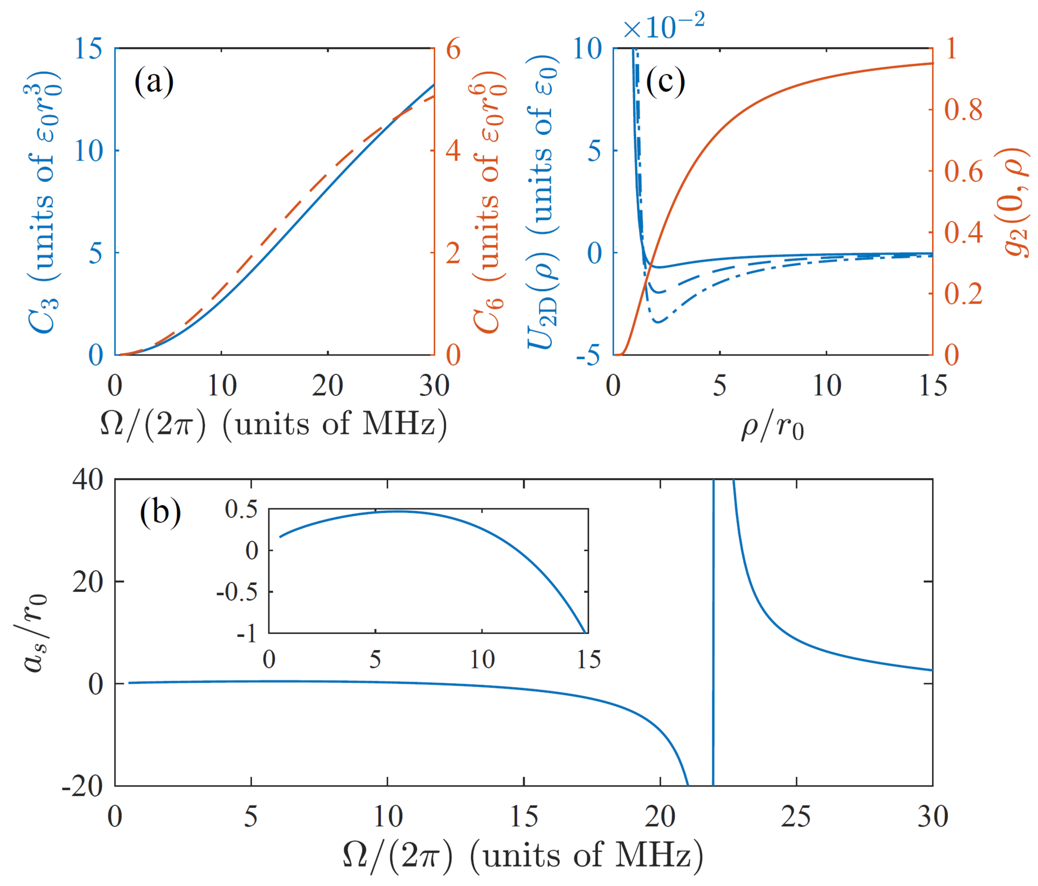
Implementation

We concentrate on the quasi-2D geometries, where the axial trap frequency is sufficiently strong such that the motion of the molecules along the z axis is frozen to the ground state of the axial harmonic oscillator, $\phi_z(z) = e^{-z^2/(2a_z^2)}/(\pi^{1/4}a_z^{1/2})$. The quasi-2D interaction is obtained by $U_{2D}(\boldsymbol{\rho}-\boldsymbol{\rho}') = \int dz dz' U(\mathbf{r}-\mathbf{r}')\phi_z^2(z)\phi_z^2(z')$. Moreover, we also solve GPE with the pseudo-potential $U_{\rm pp}(\mathbf{r}) = 4\pi\hbar^2 a_s\delta(\mathbf{r})/M + C_3(3\cos^2\theta-1)/r^3$ to illustrate drastic distinctions between molecular gases and atomic BECs.

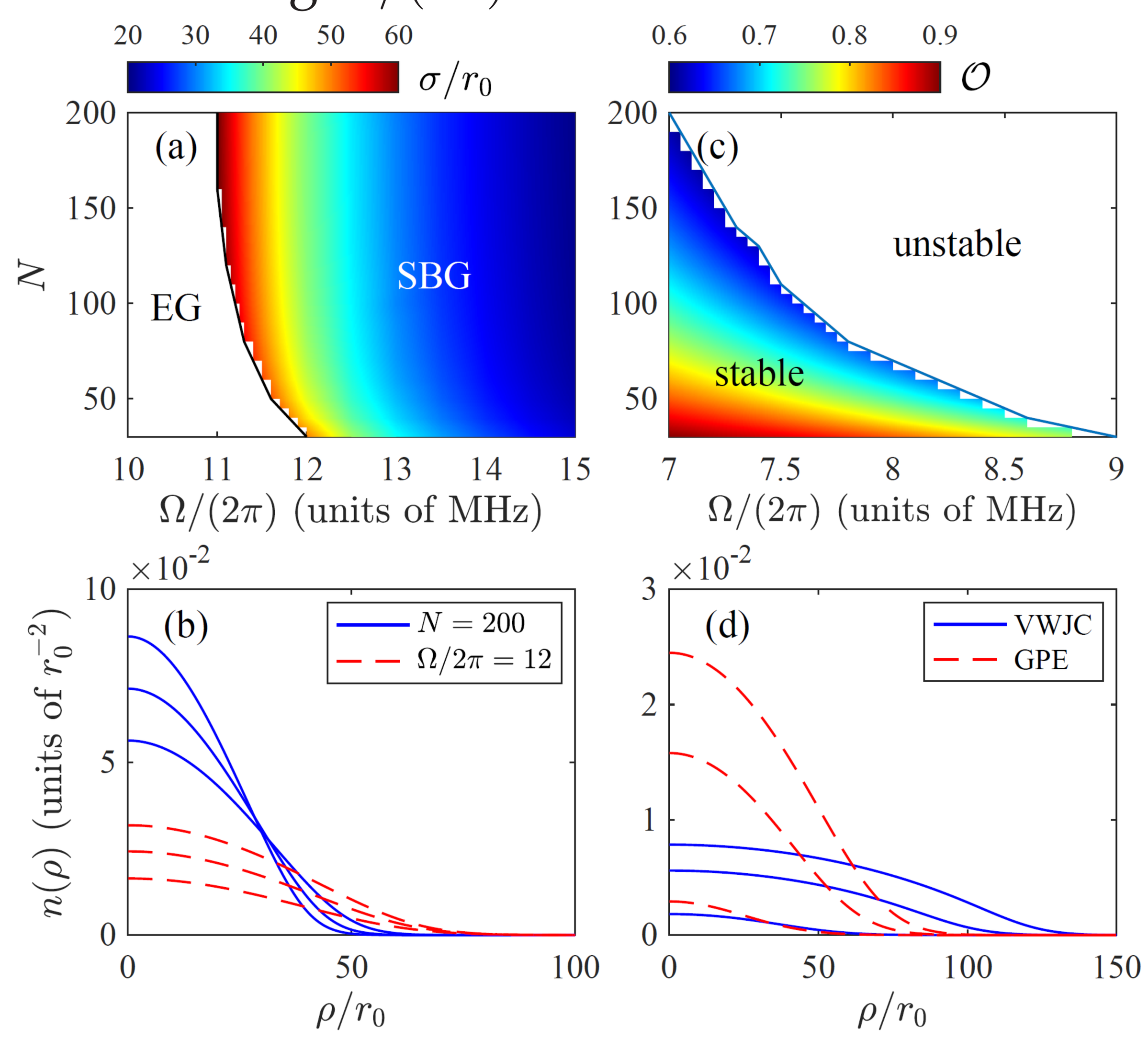
References

[1] W.-J. Jin *et al.*, Phys. Rev. Lett. **134**, 233003 (2025).

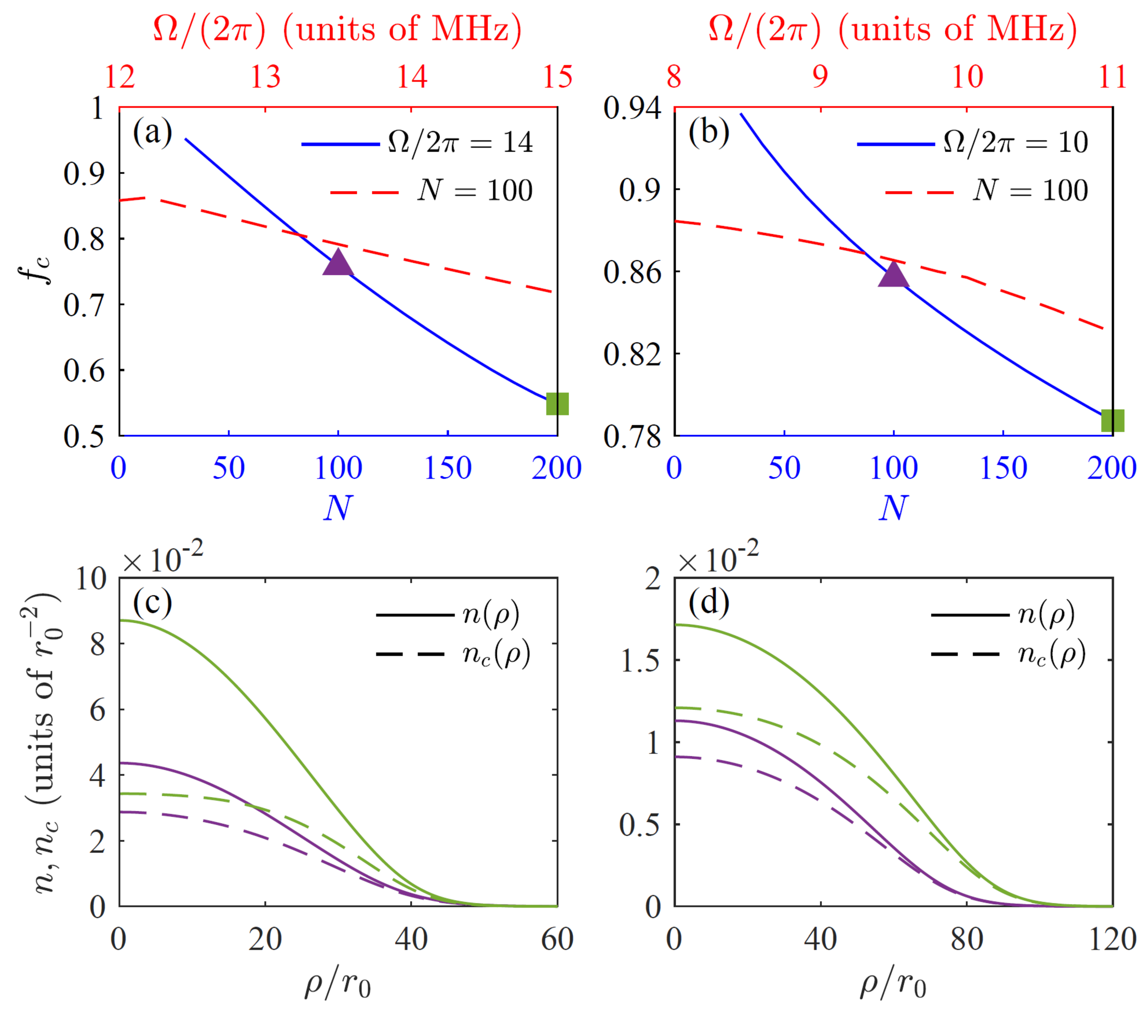
Results



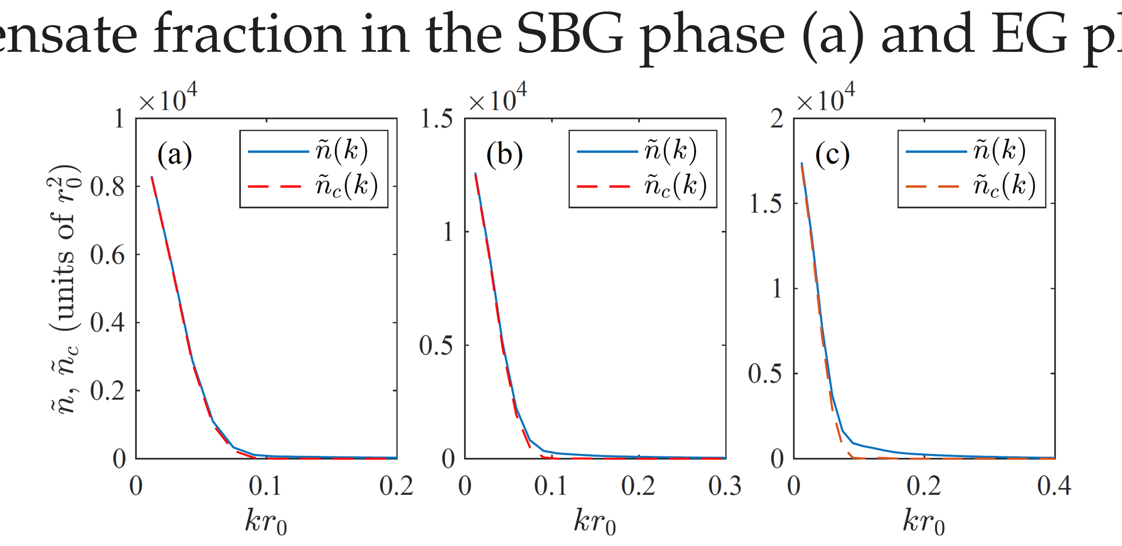
- Two-body interactions for MWS NaRb molecules with microwave detuning $\Delta/(2\pi) = 30$MHz.



- (a) Phase diagram obtained via VWJC. The colormap is the radial size of the densities. (b) Densities. Solid lines: $N = 200$ with $\Omega/(2\pi) = 14, 13.5$ and 13MHz. Dashed lines: $\Omega/(2\pi) = 12$MHz with $N = 200, 150$, and 100. (c) Stability diagram obtained via GPE. The colormap is the overlap between the densities obtained via GPE and VWJC. (d) Comparison of the total densities for $\Omega/(2\pi) = 5$MHz with $N = 200, 100$, and 10.



- Condensate fraction in the SBG phase (a) and EG phase (b).



- $\tilde{n}(k)$ and $\tilde{n}_c(k)$ for $\Omega/(2\pi) = 14$MHz with $N = 50$, 100, and 200.

Acknowledgments

This work was supported by NSFC and NKRDPC.