Supplemental Material for "Stable dilute supersolid of two-dimensional dipolar bosons"

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In the Supplemental Material we first derive explicit expressions for the energy functionals of the triangular and stripe supersolid states, in particular the expressions for the functions $\mathcal{C}_{T(S)}$, $\mathcal{D}_{T(S)}$, and $\mathcal{T}_{T(S)}$. The second part of the Supplemental Material is dedicated to the description of our numerical procedure of minimizing the grand potential density.

Derivation of the energy functionals for the triangular and stripe supersolid states

For calculating the energy functional we replace the field operators $\hat{\psi}(\mathbf{r})$ in the Hamiltonian (1) of the system with the condensate wavefunction $\psi_T(\mathbf{r})$ (7) for the triangular supersolid and with $\psi_S(\mathbf{r})$ (8) for the stripe phase. In both cases the kinetic energy term proves to be

$$\mathcal{K} = -\int d^2r \psi^*_{T(S)}(\mathbf{r}) \frac{\hbar^2\nabla^2}{2m} \psi_{T(S)}(\mathbf{r}) = \frac{\hbar^2 k^2 n}{2m} \sin^2\theta. \tag{S1}$$

In the calculation of the contribution of the two-body interaction we use the effective momentum-dependent interaction amplitude of Eq.(2). Substituting this amplitude into equation (3) in which the field operators $\hat{\psi}(\mathbf{r})$ are replaced with the condensate wavefunction $\psi_{T(S)}(\mathbf{r})$ we obtain:

$$\mathcal{H}_2^{T(S)} = \mathcal{H}_{2c}^{T(S)} + \mathcal{H}_{2d}^{T(S)}, \tag{S2}$$

$$\mathcal{H}_{2c}^{T(S)} = \frac{g_2}{2}\int d^2r |\psi_{T(S)}(\mathbf{r})|^4, \tag{S3}$$

$$\mathcal{H}_{2d}^{T(S)} = \frac{1}{2}\int d^2r |\psi_{T(S)}(\mathbf{r})|^2 f(|\mathbf{r}-\mathbf{r}'|) |\psi_{T(S)}(\mathbf{r}')|^2, \tag{S4}$$

where Eqs. (S3) and (S4) represent the contributions of the contact and dipole-dipole interactions, respectively, and the function $f(|\mathbf{r}-\mathbf{r}'|)$ writes:

$$f(|\mathbf{r}-\mathbf{r}'|) = -\pi d^2 \int \frac{d^2q}{(2\pi)^2} q \exp(i\mathbf{q}(\mathbf{r}-\mathbf{r}')). \tag{S5}$$

The integration yields:

$$\mathcal{H}_{2c}^{T(S)} = g_2 n^2 \mathcal{C}_{T(S)}(\theta), \tag{S6}$$

$$\mathcal{H}_{2d}^{T(S)} = -4\pi n^2 d^2 k \mathcal{D}_{T(S)}(\theta). \tag{S7}$$

For the triangular phase the functions $\mathcal{C}_T(\theta)$ and $\mathcal{D}_T(\theta)$ are given by

$$\mathcal{C}_T(\theta) = \frac{1}{2}\left(\cos^4\theta + 6\cos^2\theta\sin^2\theta + 4\sqrt{\frac{2}{3}}\cos\theta\sin^3\theta + \frac{5}{2}\sin^4\theta\right), \tag{S8}$$

$$\mathcal{D}_T(\theta) = \left[\cos^2\theta + \sqrt{\frac{2}{3}}\cos\theta\sin\theta + \left(\frac{1}{4} + \frac{1}{2\sqrt{3}}\right)\sin^2\theta\right], \tag{S9}$$

and for the stripe phase we have:

$$\mathcal{C}_S(\theta) = \frac{1}{2}\left(1 + 4\sin^2\theta\cos^2\theta + \frac{1}{2}\sin^4\theta\right), \tag{S10}$$

$$\mathcal{D}_S(\theta) = \left(1 - \frac{3}{4}\sin^2\theta\right). \tag{S11}$$

The integration of the third term of Eq.(1), representing the contribution of the three-body contact interaction,

$$\mathcal{H}_3^{T(S)} = \frac{g_3}{6}\int d^2r |\psi_{T(S)}(\mathbf{r})|^6, \tag{S12}$$

leads to

$$\mathcal{H}_3^{T(S)} = g_3 n^3 \mathcal{T}_{T(S)}(\theta). \tag{S13}$$

The expressions for the functions $\mathcal{T}_T$ and $\mathcal{T}_S$ read:

$$\mathcal{T}_T(\theta) = \frac{1}{6}\left(\cos^6\theta + 15\cos^4\theta\sin^2\theta + 20\sqrt{\frac{2}{3}}\cos^3\theta\sin^3\theta + \frac{75}{2}\cos^2\theta\sin^4\theta + 30\sqrt{\frac{2}{3}}\cos\theta\sin^5\theta + \frac{85}{9}\sin^6\theta\right). \tag{S14}$$

$$\mathcal{T}_S(\theta) = \frac{1}{6}\left(1 + 12\sin^2\theta - \frac{9}{2}\sin^4\theta - 6\sin^6\theta\right). \tag{S15}$$

The summation of $\mathcal{K}$ (S1), $\mathcal{H}_{2c}^i$ (S6), $\mathcal{H}_{2d}^i$ (S7), and $\mathcal{H}_3^i$ (S13), where the symbol i stands for T and S, leads to the energy functional in the form (9).

Numerical procedure

The numerical calculation is performed in the grand canonical ensemble, with a given chemical potential μ and fixed volume of the system $V = L_x L_y$. The field operator $\hat{\psi}$ is treated as a classical field, and is discretized on a two-dimensional grid with periodic boundary conditions in the coordinate and momentum space. The grand potential reads:

$$\begin{aligned}\Omega[\psi^*,\psi] = &\int d^2r\,\psi^*(\mathbf{r})h_0\psi(\mathbf{r}) + \frac{1}{2}\int d^2r\,d^2r'\,f(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2|\psi(\mathbf{r})|^2 \\ &+ \frac{g_2}{2}\int d^2r\,|\psi(\mathbf{r})|^4 + \frac{g_3}{6}\int d^2r\,|\psi(\mathbf{r})|^6 - \mu\int d^2r\,|\psi(\mathbf{r})|^2,\end{aligned} \tag{S16}$$

where the single-particle Hamiltonian h_0 includes a possible presence of the harmonic trapping potential:

$$h_0 = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2. \tag{S17}$$

The number of grid points that we use along each direction ranges from 64 to 128 in the absence of the trapping potential and from 512 to 1024 in presence of an isotropic harmonic trap.

The ground state is determined by minimizing the grand potential (S16) with the use of the *conjugate gradient* algorithm [S1]. An ingredient of this method is the line minimization, that is in each iteration the wavefunction is changed as

$$\psi_{i+1}(\mathbf{r}) = \psi_i(\mathbf{r}) + \lambda\Delta\bar{\psi}_i(\mathbf{r}), \tag{S18}$$

where $\psi_i(\mathbf{r})$ is the wavefunction in a current step, and λ is a real parameter chosen to minimize (S16) along the proposed direction $\Delta\bar{\psi}_i(\mathbf{r})$. This procedure allows us to find the global minimum encountered when moving downhill in $\Omega[\psi^*,\psi]$ along a line. Consequently, it improves the efficiency of the calculation. The direction along which to move $\psi_i(\mathbf{r})$ is constructed as

$$\Delta\bar{\psi}_i(\mathbf{r}) = \Delta\psi_i(\mathbf{r}) + \frac{\int d^2r\,\Delta\psi_i^*(\mathbf{r})\left[\Delta\psi_i(\mathbf{r}) - \Delta\psi_{i-1}(\mathbf{r})\right]}{\int d^2r\,|\Delta\psi_{i-1}(\mathbf{r})|^2}\Delta\bar{\psi}_{i-1}(\mathbf{r}), \tag{S19}$$

in order to be *conjugate* with respect to the direction $\Delta\bar{\psi}_{i-1}(\mathbf{r})$ used in the previous step, and

$$\Delta\psi_i(\mathbf{r}) = -\frac{\delta\Omega}{\delta\psi^*} = -\left[\mathcal{H}_{\rm GP}(\mathbf{r}) - \mu\right]\psi_i(\mathbf{r}), \tag{S20}$$

is the gradient of the functional $\Omega[\psi^*,\psi]$ evaluated with $\psi_i(\mathbf{r})$, where

$$\mathcal{H}_{\rm GP} = h_0 + \int d^2r'\,f(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + g_2|\psi(\mathbf{r})|^2 + \frac{g_3}{2}|\psi(\mathbf{r})|^4 \tag{S21}$$

is the Gross-Pitaevskii Hamiltonian. The integral in the second term of Eq. (S21) can be calculated by using the convolution theorem [S2], namely

$$\int d^2r'\, f(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 = \mathcal{F}^{-1}\left\{\mathcal{F}\left[f\right](\mathbf{q})\,\mathcal{F}\left[|\psi|^2\right](\mathbf{q})\right\} \tag{S22}$$

where $\mathcal{F}\left[f\right](\mathbf{q})$ and $\mathcal{F}\left[|\psi|^2\right](\mathbf{q})$ are the Fourier transforms of $f(\mathbf{r})$ and $|\psi(\mathbf{r})|^2$ respectively, and $\mathcal{F}^{-1}$ is the inverse transform. We set that the convergence is reached when the relative difference in the grand potential between the neighboring time steps is smaller than 5×10^{-9}.

In the absence of external trapping, the wave function can remain finite at the boundary. Due to the periodic boundary condition, the structure of the modulation for a non-uniform state is then limited by the size of the system imposed in the simulation. In order to overcome this constraint, for each given set of parameters (g_2, g_3, d, μ) we run the simulation several times with different L_x and L_y ranging from $4\pi/k_m$ to $9\pi/k_m$ respectively, where $k_m = 4\pi n r_* \mathcal{D}_{T(S)}(\theta)$ is fixed by the variational ansatz. In the end we choose the ground state as the one corresponding to the lowest grand potential density Ω/V.

Different trial wavefunctions are used in the simulation, including a uniform state, triangular (hexagonal) lattice state, square lattice state, stripe state, a combination of triangular (hexagonal) and stripe states. This is done in order to check whether the final result is biased by the initial conditions or not. We have also compared with each other the results obtained with a different number of grid points to make sure that they are not affected by the discretization of space.

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