TOTAL SPIN OF THE HF-STATES

Without imposing the polarization, each ρ_k may be written as a matrix

$$\rho_k(q,q') = \begin{pmatrix} \rho_{k,\uparrow\uparrow}(q,q') & \rho_{k,\uparrow\downarrow}(q,q') \\ \rho^*_{k,\uparrow\downarrow}(q,q') & \rho_{k,\downarrow\downarrow}(q,q') \end{pmatrix} \tag{1}$$

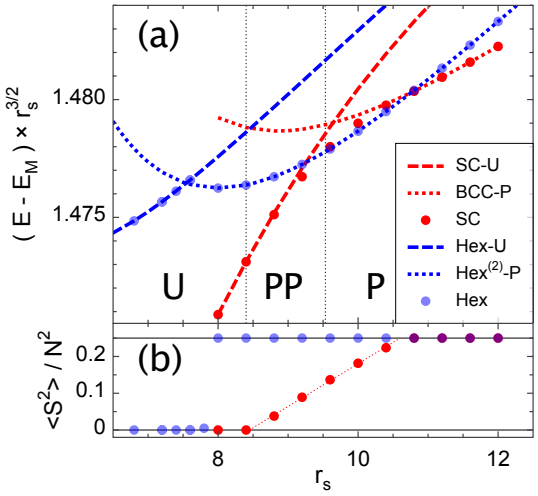
The total spin square reads $S^2 = \sum_{\alpha=1}^{3} (\sum_i s_i^\alpha)^2$ where s_i^α are the components of the spin of particle i, and we have

$$s^2 = \frac{\langle S^2 \rangle}{N^2} = \frac{1}{N^2} \mathbf{Tr}\, S^2 \rho_N = \frac{N-1}{N} \sum_{a=1}^{3} \mathbf{Tr}\, \rho_2 s^\alpha \otimes s^\alpha + \frac{3}{4N} \tag{2}$$

Inserting Eq. (1) of the main text, we get in the thermodynamic limit (the exchange term vanishes):

$$s^2 \underset{N\to\infty}{\longrightarrow} \sum_{\alpha=1}^{3} (\mathbf{Tr}\, \rho_1 s^\alpha)^2 = \frac{(\mathbf{Tr}\, \rho_{\uparrow\uparrow} - \mathbf{Tr}\, \rho_{\downarrow\downarrow})^2}{4} + |\mathbf{Tr}\, \rho_{\uparrow\downarrow}|^2 \tag{3}$$

The polarized case (P), $s^2 = 1/4$, can be obtained with various total spin orientation. One can show that after a rotation, one has $\mathbf{Tr}\, \rho_{\uparrow\uparrow} = 1$ and $\mathbf{Tr}\, \rho_{\downarrow\downarrow} = \mathbf{Tr}\, \rho_{\uparrow\downarrow} = 0$. The unpolarized case, $s^2 = 0$ is obtained with $\mathbf{Tr}\, \rho_{\uparrow\uparrow} = \mathbf{Tr}\, \rho_{\downarrow\downarrow}$ (same number of up and down spins) and $\mathbf{Tr}\, \rho_{\uparrow\downarrow} = 0$. Many states are possible where $\rho_{\uparrow\downarrow} \neq 0$. In the paper, unpolarized states (U) means $\rho_{\uparrow\downarrow} = 0$. Here, we call restricted the U and P states and unrestricted the general model (Eq.1).



		E (mHa)		
r_s	$\langle S^2 \rangle / N^2$	unrestricted	U	P
8.0	0.0000	-46.987	-46.987	-46.618
8.4	0.0000	-46.150	-46.150	-45.916
8.8	0.0379	-45.303	-45.301	-45.167
9.2	0.0891	-44.464	-44.451	-44.392
9.6	0.1367	-43.636	-43.608	-43.603
10.0	0.1815	-42.823	-42.777	-42.812
10.4	0.2238	-42.026	-41.961	-42.025
10.8	0.2500	-41.247	-41.164	-41.247
11.2	0.2500	-40.483	-40.386	-40.483
11.6	0.2500	-39.734	-39.629	-39.734
12.0	0.2500	-39.003	-38.893	-39.003

FIG. 1. Results with $M = 16$ for SC symmetry in red ($M_\Lambda = 57$), Hex symmetry in blue ($M_\Lambda = 35$). Dashed and dotted lines and circles stand for U, P, and the unrestricted model, respectively. (a): Energy versus r_s, $E_M = 0.89593/r_s$ is the P-BCC Madelung energy. Vertical dotted lines separate the domains where the overall ground state is unpolarized (U), polarized (P) or the partially polarized one (PP). (b): $\langle S^2 \rangle / N^2$ (see Eq.3) versus r_s. The red dotted line is a linear fit through the partially polarized points. Energies per particle and $\langle S^2 \rangle / N^2$ for SC symmetries are summarized in the table.

The phase diagram, Fig. 3 of the main article has been obtained with restricted (U and P) states. Since the U-P transition happens around the density region $8 < r_s < 12$, we focus on it by performing unrestricted calculations. With SC symmetry (leading to solutions with BCC charge symmetry), we can follow the transition from U-SC to P-BCC. Fig.1-a shows the energies versus r_s all models. Fig.1-b shows the variations of s^2 where a crossover is seen for $8.5 < r_s < 10.6$, the domain where the unrestricted model leads to lower energy states than the restricted ones. The other candidate for the absolute ground state is with Hex symmetry where the ground state goes for U-Hex directly to P-Hex$^{(2)}$ (see Fig.1a-b). The comparison of all these curves shows a transition for U-SC to P-Hex$^{(2)}$ within a small region ($8.4 < r_s < 9.5$) where the polarization of the SC phase increases. More work is under investigation to understand this partially polarized phase.

For the remaining U-BCC, U-FCC, U-Hex$^{(2)}$ symmetries, we have checked on small system ($M = 8$) that the unrestricted results do not improve the energies.

GROUND STATE ENERGIES VERSUS r_s

Unpolarized				
r_s	E(mHa)	ΔE(mHa)	Q/k_F	sym.
3.0	-29.954	-0.005	1.9495	IC-bcc
3.1	-32.826	-0.010	1.9456	IC-bcc
3.2	-35.289	-0.017	1.9406	IC-bcc
3.3	-37.399	-0.026	1.9341	IC-bcc
3.4	-39.287	-0.117	0.8794	Hex$^{(2)}$
3.5	-40.923	-0.272	0.8794	Hex$^{(2)}$
3.6	-42.437	-0.427	0.8794	Hex$^{(2)}$
3.7	-43.727	-0.611	1.7589	fcc
3.8	-44.899	-0.849	1.7589	fcc
4.0	-46.775	-1.293	1.7589	fcc
4.2	-48.157	-1.709	1.7589	fcc
4.4	-49.151	-2.096	1.7589	fcc
4.6	-49.841	-2.459	1.7589	fcc
4.8	-50.292	-2.799	1.7589	fcc
5.0	-50.554	-3.119	1.7589	fcc
5.2	-50.665	-3.420	1.7589	fcc
5.4	-50.656	-3.703	1.7589	fcc
5.6	-50.551	-3.970	1.7589	fcc

Unpolarized				
r_s	E(mHa)	ΔE(mHa)	Q/k_F	sym.
5.8	-50.368	-4.221	1.7589	fcc
6.0	-50.192	-4.524	1.6120	sc
6.2	-50.031	-4.878	1.6120	sc
6.4	-49.813	-5.201	1.6120	sc
6.6	-49.550	-5.497	1.6120	sc
6.8	-49.249	-5.768	1.6120	sc
7.0	-48.919	-6.017	1.6120	sc
7.2	-48.566	-6.247	1.6120	sc
7.4	-48.193	-6.457	1.6120	sc
7.6	-47.804	-6.649	1.6120	sc
7.8	-47.403	-6.825	1.6120	sc
8.0	-46.992	-6.987	1.6120	sc
8.2	-46.576	-7.135	1.6120	sc
8.4	-46.155	-7.271	1.6120	sc
8.6	-45.731	-7.396	1.6120	sc
8.8	-45.307	-7.511	1.6120	sc
9.0	-44.883	-7.617	1.6120	sc
9.2	-44.461	-7.716	1.6120	sc

Polarized				
r_s	E(mHa)	ΔE(mHa)	Q/k_F	sym.
9.4	-44.050	-7.814	0.8794	Hex$^{(2)}$
9.6	-43.647	-7.911	0.8794	Hex$^{(2)}$
9.8	-43.245	-7.998	0.8794	Hex$^{(2)}$
10.0	-42.844	-8.077	0.8794	Hex$^{(2)}$
10.2	-42.444	-8.146	0.8794	Hex$^{(2)}$
10.4	-42.047	-2.759	1.7589	fcc
10.7	-41.461	-2.833	1.7589	fcc
11.0	-40.883	-2.901	1.7589	fcc
11.5	-39.936	-3.003	1.7589	fcc
12.0	-39.015	-3.092	1.7589	fcc
12.5	-38.126	-3.171	1.7589	fcc
13.0	-37.267	-3.242	1.7589	fcc
13.5	-36.441	-3.306	1.8094	bcc
14.0	-35.645	-3.362	1.8094	bcc
14.5	-34.880	-3.412	1.8094	bcc
15.0	-34.142	-3.455	1.8094	bcc
15.5	-33.432	-3.491	1.8094	bcc
16.0	-32.748	-3.522	1.8094	bcc

TABLE I. Ground state energies, E, at the thermodynamic limit, in milli-Hartree units (mHa) and energy gain, $\Delta E = E - E_{FG}$, compared to the Fermi gas solution (precision: ~ 5 on the last digit) Q is the modulus of the generator of Λ (see Eq. (2) of the main article). sym. means lattice symmetry. IC indicates incommensurate crystalline order.

Following are details on the size effects as defined in Eqs. 4-5 of the main text. We recall:

$$E_M^{(1)} = -\frac{\alpha\gamma Q C_\Lambda}{4\pi r_s M} \tag{4}$$

$$E_M^{(2)} = -\frac{\gamma Q S_0}{\pi M}\ E_M^{(1)} \tag{5}$$

where $\alpha^3 = 9\pi/(2n_s)$, $\gamma^3 = \det(M_Q)$ and C_Λ, the Madelung constant, are given in the Tab. II, and $S_0 = \lim_{\mathbf{k}\to 0} S(\mathbf{k})/\|\mathbf{k}\|$. S_0 is given in Tab. III for the incommensurate phase (IC-bcc) and $S_0 = 0$ in the Wigner phase ($Q = Q_W$).

lattice	sc	bcc	fcc	Hex	Hex$^{(2)}$
n_c	1	1	1	1	2
M_Q	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	$\frac{1}{\sqrt{3}}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$	$\frac{4\sqrt{2}}{3}\begin{pmatrix} 1 & 1/2 & 0 \\ 0 & \sqrt{3}/2 & 0 \\ 0 & 0 & 3/(4\sqrt{2}) \end{pmatrix}$	
γ^3	1	$\frac{1}{\sqrt{2}}$	$\frac{4}{3\sqrt{3}}$	$\frac{16}{3\sqrt{3}}$	
Q_W/k_F	1.611991954016	1.809399790564	1.758882522024	1.108026556895	0.879441261012
C_Λ	-2.837297479481	-2.888461503054	-2.888282119020	-2.512880623796	

TABLE II. Lattice definitions and properties. n_c is the number of electrons per primitive cell. $M_Q = (\mathbf{Q}_1/Q, \mathbf{Q}_2/Q, \mathbf{Q}_3/Q)$. For the hexagonal case, $Q = \|\mathbf{Q}_3\|$. Q_W is given by: $Q_W/k_F = \gamma(4\pi/(3n_c))^{1/3}$, $k_F = \alpha/r_s(a.u.)$.

r_s	3.0	3.1	3.2	3.3
$S_0 k_F$	0.596(5)	0.567(5)	0.540(5)	0.512(5)

TABLE III. $S_0 = \lim_{\mathbf{k}\to 0} S(\mathbf{k})/\|\mathbf{k}\|$ versus r_s for IC-U-bcc.