Supplementary Information for

Collective inter-layer pairing and pair-superfluidity in vertically-stacked layers of dipolar excitons

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S1. Additional QMC data

In this section, we provide additional numerical results supporting the ones appearing in the main text. We begin by computing the evolution of inter- and intra-layer density-density correlation functions for varying density imbalances. In Fig. S1(a) and Fig. S1(b), we plot $g_{11}(r)$ and $g_{12}(r)$, respectively, for several values of $\gamma$ at $L_z = 0.3[a]$ and $n_1 = 0.83[a^{-2}]$, corresponding to the PSF phase at $\gamma = 0$. We find that density imbalance smears the correlation peaks appearing both in $g_{11}(r)$ and $g_{12}(r)$. At large density imbalances, intra-layer correlations eventually vanish and $g_{11}(r)$ approaches the monolayer result, shown with a dashed line in Fig. S1(a). To understand this effect, we note that paired dipoles are heavier and carry enlarged effective dipole moment, compared to independent dipoles. Hence, their kinetic energy is quenched and the repulsion between them is amplified, promoting spatial correlations as a precursor of a crystalline phase. In Fig. S1(c), we depict the effective IX dipole sizes for the proposed GaAs-based bilayer DQW structure, described in the main text. Here, we calculate the effective IX dipole sizes for the proposed GaAs-based bilayer DQW structure, described in the main text. Moreover, the predicted energy shifts in TMD materials are considerably larger in the experimentally relevant regimes. We consider both GaAs and TMD based heterostructures with layer separations $L_z = 44[\text{nm}]$ and $L_z = 9[\text{nm}]$, respectively, as proposed in the main text. We find that $\Delta \mu_1$ increases with decreasing density and saturates in the dilute limit, see Fig. S6. Moreover, the predicted energy shifts in TMD materials are considerably larger compared to the GaAs case, as discussed in the main text.

S2. Single IX solution

Here, we calculate the effective IX dipole sizes for the proposed GaAs-based bilayer DQW structure, described in the main text. To that end, we numerically solve the single particle Schrödinger equation for the electron and hole, taking relative permittivity $\varepsilon = 12.9$ and including an externally applied electric field $F_z$. In Fig. S7, we depict the electron and hole states, $\psi_n^{e(h)}$, along the stacking direction, $z$, for electric field $F_z = -2.5[\text{V/\mu m}]$. We find that the external field enhances IX dipole sizes in both layers relative to the zero voltage case, giving an increased effective dipole size $d = 22[\text{nm}]$. We now proceed to monitor the finite size and finite temperature convergence of our numerical data. In Fig. S4, we depict the evolution of inter- and intra-layer density-density correlation functions for varying density imbalances. We obtain a similar result for $40(5)$. These results corroborates the predicted scaling behavior.

Next, in Fig. S3, we present a finite size scaling analysis of the two step BKT transitions, separating the normal to PSF and PSF+layer-$\alpha$ SF phases, at finite density imbalance $\gamma = 0.125$, and for $L_z = 0.2[a]$ and $n_1 = 1.23[a^{-2}]$. As in the main text, following the standard Nelson jump criterion (3) $\rho_\pm(T = T_c) = \frac{\nu}{2} T_c$, we search for the crossings of $\rho_\pm$ curves and the line $\frac{\nu}{2} T$. We find good agreement among crossing temperatures belonging to different systems sizes, allowing for an accurate determination of the BKT transition temperatures.

We now proceed to monitor the finite size and finite temperature convergence of our numerical data. In Fig. S4, we depict the dependence of the total energy per particle, $\epsilon = E/(N_1 + N_2)$, and superfluid stiffness, $\rho_-$, on density imbalance for $L_z = 0.3[a]$, $n_1 = 0.83[a^{-2}]$, $N_1 = 32$ and a set of decreasing temperatures. We indeed observe convergence to the ground state value for the lowest temperature considered, $T = 0.08[E_0]$. In Fig. S5, we again plot $\epsilon$ and $\rho_-$ as a function of $\gamma$ for an increasing range of system sizes at $L_z = 0.3[a]$, $n_1 = 0.83[a^{-2}]$ and temperature $T = 0.08[E_0]$. From the clear convergence of the curves, we can safely deduce that $N_1 = 32$ is sufficiently large to represent the thermodynamic limit result.

Lastly, we estimate the IX energy shift given by the jump discontinuity in the chemical potential, $\Delta \mu_1$, for several IX densities in the experimentally relevant regimes. We consider both GaAs and TMD based heterostructures with layer separations $L_z = 44[\text{nm}]$ and $L_z = 9[\text{nm}]$, respectively, as proposed in the main text. We find that $\Delta \mu_1$ increases with decreasing density and saturates in the dilute limit, see Fig. S6. Moreover, the predicted energy shifts in TMD materials are considerably larger compared to the GaAs case, as discussed in the main text.
Fig. S1. (a) Intra- and (b) inter-layer density-density correlation function plotted for several $\gamma$ values for $L_z = 0.3[a]$ and $n_1 = 0.83[a^{-2}]$. The black dashed line in (a) corresponds to a single layer of two-dimensional dipolar bosons. (c) Zero separation limit of $g_{12}(r)$ as a function of $\gamma$ at $L_z = 0.3[a]$. Density values $n_1$ residing in the PSF (2SF) phase at equal densities are shown by dashed (solid) lines. These results were obtained at $T = 0.08[E_0]$ and $N_1 = 32$. 
Fig. S2. Universal curve collapse analysis of (a) the jump discontinuity, $\Delta \mu_1$, and (b) superfluid stiffness in the SCF channel, $\rho_\nu$, near the critical point $n_{c1}$ for the PSF to 2SF transition. Different colors correspond to different system sizes. Results are shown for $T = 0.08|E_0|$ and $L_z = 0.4|a|$. 
Fig. S3. (a) $\rho_+$ and (b) $\rho_-$ as a function of the temperature, for several system sizes. The black line corresponds to the Nelson criterion $\pi T/2$. In the above figures we set $L_z = 0.2 [a]$, $n_1 = 1.23 [a^{-3}]$ and $\gamma = 0.125$. 

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Fig. S4. Zero temperature convergence of (a) $\epsilon$ and (b) $\rho_-$ as a function of $\gamma$. Here, we set $L_z = 0.3[a]$, $n_1 = 0.83[a^{-2}]$ and $N_1 = 32$. 
Fig. S5. Finite size convergence of (a) $\epsilon$ and (b) $\rho_-$ as a function of $\gamma$ at $L_z = 0.3[a]$, $n_1 = 0.83[a^{-2}]$ and $T = 0.08[E_0]$. 
Fig. S6. IX energy shifts as a function of IX densities. Blue and red colors correspond to the GaAs and TMD based settings described in the main text, respectively. The corresponding layer separations of both structures are denoted in the legend. These results were obtained in the ground state limit with $N_1 = 32$ and $N_2 = 16$ for the GaAs and TMD curves, respectively.
**Fig. S7.** IX states in bilayer DQW potential in the presence of an external electric field $F_e = -2.5$ [V/µm]. The upper and lower black lines correspond to the conduction and valance band given by the bilayer DQW structure, respectively. The blue and red curves correspond to the electron (solid line) and hole (dashed line) wavefunctions at layer $\alpha = 1, 2$, respectively.

**References**

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