RVB superconductors with fermionic projected entangled pair states: *supplemental material*

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DENSITY-DENSITY CORRELATIONS AND COULOMB ENERGY

Superconducting (Cooper) pairs are bound states of charged electrons (or holes) and, hence, are expected to be destabilized by strong short range (SR) Coulomb repulsion. In cuprates superconductors the NN repulsion V_1 between doped holes is expected to be large, typically $V_1 \sim t$ or larger [1], and the superconducting coherence length is short. It is therefore interesting to investigate the related energy cost in a RVB superconductor. One can take into account the SR Coulomb repulsion by adding to the (extended) t–J model a term like:

$$H_{\mathrm{V}} = V_1 \sum_{\langle ij \rangle} (n_i - x)(n_j - x) + V_2 \sum_{\langle\langle kl \rangle\rangle} (n_k - x)(n_l - x) + \cdots \tag{1}$$

where $n_i = 1 - c_{i\sigma}^{\dagger} c_{i\sigma}$ is the local hole density operator and the repulsion beyond NN ($V_1 > 0$) and NNN ($V_2 > 0$) sites can safely be neglected. Note that we have subtracted the energy cost $2V_1 x^2 + 2V_2 x^2$ (per site) of an uncorrelated uniform charge background. The variational energies of both terms are therefore proportional to the corresponding *connected* density-density correlators,

$$C_{ij} = \langle (n_i - x)(n_j - x) \rangle. \tag{2}$$

The NN and NNN correlators C_{NN} and C_{NNN} are shown in Fig. 1(a) for two different RVB ansätze, (i) the $c = 0$ pure $d+is$ superconductor (with only NN pairing) and (ii) the optimized $c = -0.65$ (predominantly) d-wave superconductor. $C_{ij} > 0$ ($C_{ij} < 0$) corresponds to an enhanced (suppressed) density correlation w.r.t. a uniform background of uncorrelated holes. The strong NN correlation in the pure $s + id$ RVB superconductor is consistent with NN hole (Cooper) pairs and a superconducting coherence length of just one lattice spacing. For the optimized RVB the largest density correlation occurs between NNN sites suggesting that Cooper pairs are predominantly NNN hole pairs despite the dominant d-wave character of the pairing field, in agreement with early exact diagonalisations on small t–J clusters [2].

Short distance pairing yields an increase of Coulomb energy $2V_1 C_{NN}/x + 2V_2 C_{NNN}/x$ per hole. Each term is plotted separately in Fig. 1(b) for the two RVB wave functions studied here. Assuming $V_2 \ll V_1$, we observe that the energy cost is very much reduced in the optimized RVB compared to the reference $c = 0$ state, due to a larger coherence length (or Cooper pair size). Quantitatively, one finds a Coulomb energy of $\sim 0.04V_1$ (per hole) which remains quite small compared to the *gain* of kinetic energy $|e_k| \sim 2.5t$ (per hole), even if $V_1 > t$.

DETAILS ABOUT THE IPEPS CALCULATIONS

The (optimized) $d + is$ RVB superconductor has been compared to fermionic iPEPS calculations using the same bond dimension $D = 3$ for the same Hamiltonian parameters i.e. $J_2 = 0.5 J_1$ and $J_1/t = 0.4$ as in the paper (see Ref. [3] for an introduction to the method). We used two different optimization methods, the simple update from Ref. [4] and the full update method from Ref. [5] for Hamiltonians with next-nearest neighbor interactions. The former approach is computationally cheaper but less accurate than the latter one (see Ref. [3] for a discussion). Both optimization methods require a 2×2 unit cell of tensors (or larger) which is periodically repeated on the lattice.

Figure 2 shows that the best state obtained with the full update optimization with $D = 3$ (blue stars) is only slightly lower than the constructed $c = -0.65$ RVB state (open black circles), which is remarkable given the fact that
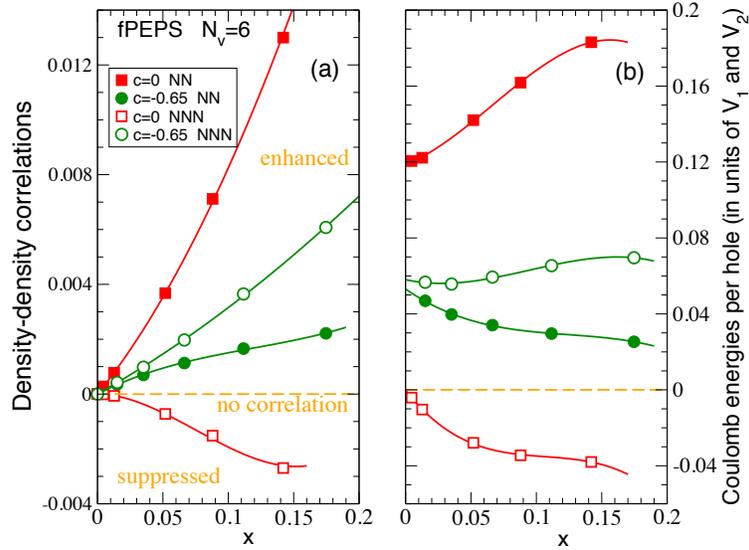
FIG. 1: (a) Density-density correlations between NN and NNN sites as a function of doping. The two RVB $d+is$ superconductors with $c = 0$ (pure $d + is$ RVB) and $c = -0.65$ (optimized RVB) are compared (computations made on an infinitely long $N_v = 6$ cylinder). (b) NN and NNN Coulomb energies per hole.
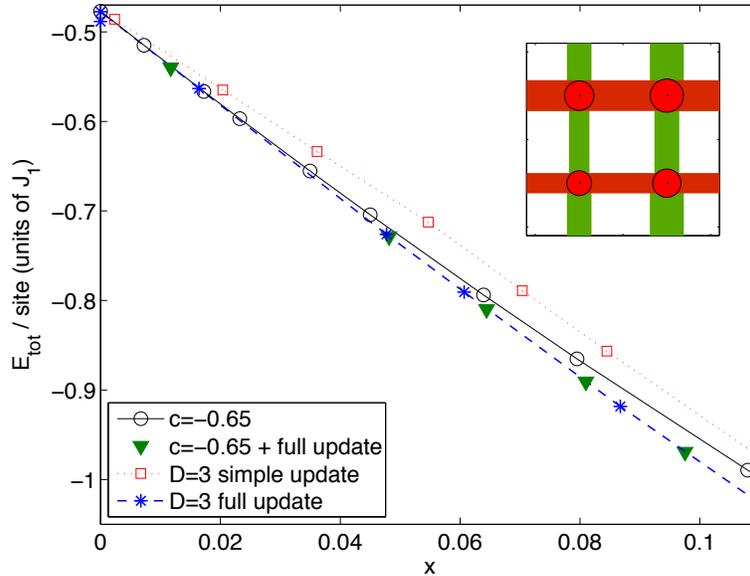

FIG. 2: Total energy (per site) of the d+is ansatz with $c = -0.65$ and the optimized $D = 3$ iPEPS wavefunctions (using different update methods and initial states) as a function of doping. Inset: Real space pattern of the best $D = 3$ iPEPS state within the 2×2 unit cell for $x = 0.091$. The red dots show the hole density, and the colored bonds the pairing amplitude with different signs.

the latter has only one single variational parameter. These results have been obtained starting from a random initial state (with the same random tensor on each lattice site), and a similar result is obtained by using the $c = -0.65$ RVB ansatz as initial state for the full optimization (green triangles). We note that depending on the random initial state some of the simulations also converged to other (competing) states, but all having a higher energy. The simple update method (red squares) fails to find the best state in this case, but yields states with a higher energy. All these results show that the (kinetic energy) optimized $d + is$ RVB state is an excellent $D = 3$ ansatz for this range of Hamiltonian parameters, and it can serve as an ideal initial state for fermionic iPEPS to study RVB phases, e.g. to

perform simulations at larger D.

We note that there is a jump in the energy per site in the iPEPS data at $x = 0$. The reason is that for $x = 0$ there are no charge degrees of freedom and the iPEPS can fully exploits its auxiliary space of dimension $D = 3$ for the spin degrees of freedom, whereas for any finite x the iPEPS needs to carry also information on the charge degrees of freedom through its auxiliary space. In other words, since for $x = 0$ there are less degrees of freedom the $D = 3$ iPEPS lies closer to the true ground state than the one at finite x, which leads to a discontinuity in the energy per site. For this reason we computed the energy per hole in the main text as $E_{hole} = (\langle H \rangle_x - \langle H \rangle_{0+\epsilon})/x$ where we take $\epsilon \to 0$. Finally we note that also the energy of the RVB ansatz for $x = 0$ can also be further improved, see Ref. [6].

An important feature of the RVB $d+is$ superconductor is that it is translationally invariant (i.e. it is uniform) and its bond SC amplitudes are invariant under all (rotation and/or reflection) symmetry operations of the lattice C_{4v} point group (although minor differences between vertical and horizontal directions occur on finite circumference cylinders due to small finite-size effects). Furthermore it preserves the SU(2) spin rotation symmetry. The best optimized iPEPS reproduces these symmetries approximately, in particular the magnetic moment at each site vanishes entirely (i.e. the SU(2) symmetry is unbroken), and there are only little variations in the hole density per site and the bond SC amplitudes (see inset of Fig. 2). This slight symmetry breaking can be partly due to the Trotter error in the optimization method and/or to the fact that a finite bond dimension can also artificially induce a symmetry breaking (which typically gets fully restored for large D).

Using larger unit cells we expect to get stripe states similarly as in the plain t–J model [7] competing with the uniform RVB superconductor. A full study using the full update is challenging (more challenging than in the plain t–J model because of the next-nearest neighbor interaction which leads to a higher computational cost) and is left for further studies.

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[1] C. J. Calzado and J.-P. Malrieu, Phys. Rev. B **63**, 214520 (2001).
[2] D. Poilblanc, Phys. Rev. B **49**, 1477 (1994).
[3] P. Corboz, R. Orus, B. Bauer, and G. Vidal, Phys. Rev. B **81**, 165104 (2010).
[4] P. Corboz, J. Jordan, and G. Vidal, Phys. Rev. B **82**, 245119 (2010).
[5] P. Corboz and F. Mila, Phys. Rev. B **87**, 115144 (2013).
[6] L. Wang, D. Poilblanc, Z.-C. Gu, X.-G. Wen, and F. Verstraete, Phys. Rev. Lett. **111**, 037202 (2013).
[7] P. Corboz, T. M. Rice, and M. Troyer, arXiv:1402.2859 [cond-mat] (2014).