Coulomb electron pairing in a tight-binding model of La-based cuprate superconductors

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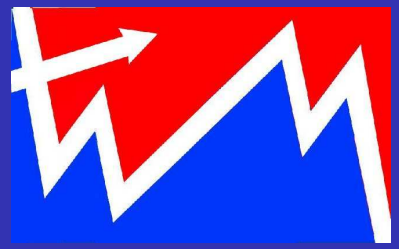
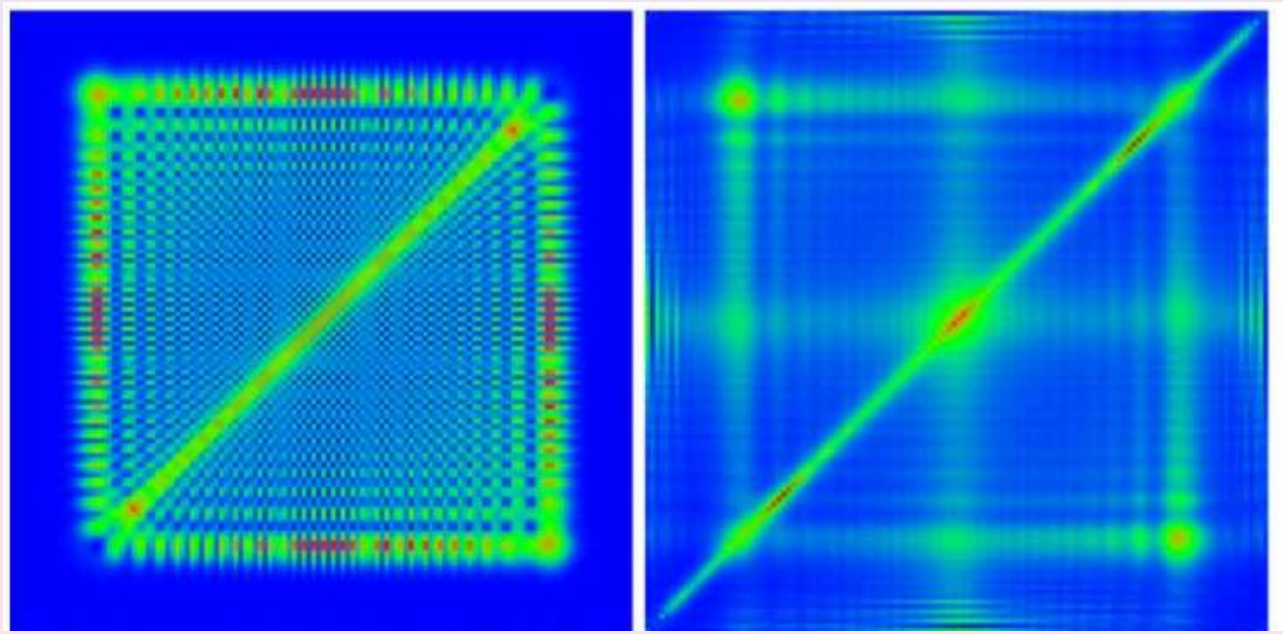


with Klaus Frahm (LPT, Univ. Paul Sabatier, Toulouse)



MAIN STATEMENT: repulsive long-range interaction creates two electron pairs in narrow band structures; PRR **2**, 023354 (2020); EPJB **94**, 29 (2021)

Support: LABEX NANOX MTDINA project (disruptive)

Ancient interest to interactions in narrow energy bands

PHYSICAL REVIEW VOLUME 137, NUMBER 6A 15 MARCH 1965

Correlation of Electrons in a Narrow *s* Band

MARTIN C. GUTZWILLER
IBM Watson Laboratory, Columbia University, New York, New York
(Received 22 October 1964)

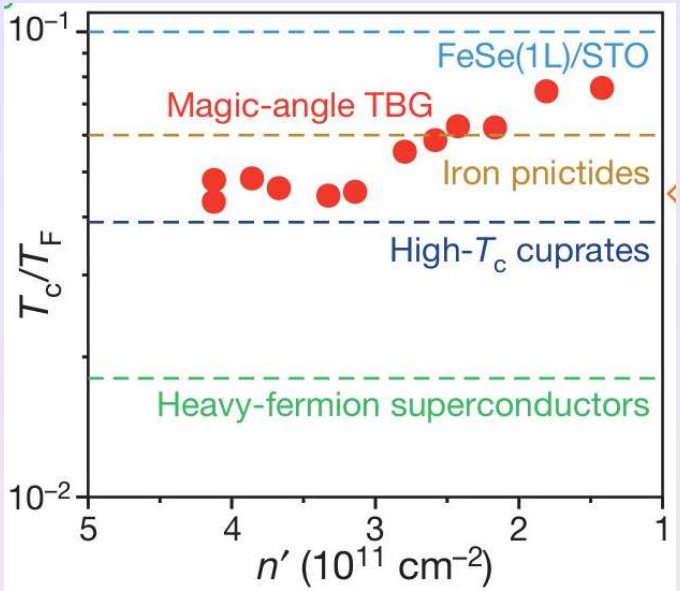
PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Electron Correlations in Narrow Energy Bands

J. Hubbard

Proc. R. Soc. Lond. A 1963 **276**, 238-257
doi: 10.1098/rspa.1963.0204

Renewed interest due to twisted bilayer graphene



from Y.Cai et al. Nature **556**, 43 (2018)

PHYSICAL REVIEW X **8,** 031088 (2018)

Symmetry, Maximally Localized Wannier States, and a Low-Energy Model for Twisted Bilayer Graphene Narrow Bands

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Narrow band structure at low energies; indications on importance of electron -electron interactions (e.g. triplet pairs Y.Cao et al Nature **595**, 526 (2021))

Tight-binding model for La-based cuprate superconductors

ORIGINAL PAPER

annalen der physik
www.ann-phys.org

A 3D Tight-Binding Model for La-Based Cuprate Superconductors

*Raphaël Photopoulos and Raymond Frésard**

Ann. Phys. (Berlin) **2019**, 1900177 (2019)

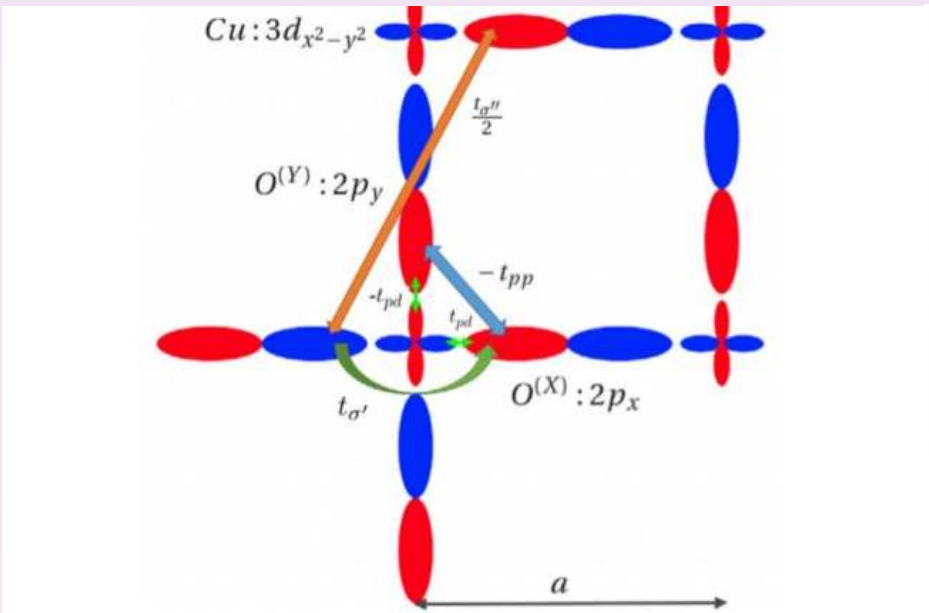


Figure 1. Illustration of t_{pd}, $t_{\sigma'}$, t_{pp}, and $t_{\sigma''}$ in-plane hopping amplitudes. Note that $t_{pp} = (t_\sigma + t_\pi)/2$ and $t_{\sigma''}$ are introduced using the rotated orbital basis $(2p_\xi^{(X,Y)}, 2p_\eta^{(X,Y)})$.

Table 2. In-plane tight-binding parameters set determined from LDA calculations or ARPES data and compared to the ones from the Emery model ($\Delta_{pd} = 3.5t_{pd}$, $t_{pp} = 0.6t_{pd}$) and this work (parameters given in Table 1).

In-plane	t	t'/t	t''/t	t'''/t	$t^{(4)}/t$
ARPES (ref. [47])	0.25 (eV)	−0.09	0.07	0.105	—
ARPES (ref. [74])	0.195 (eV)	−0.095	0.075	0.09	0.02
LDA (ref. [47])	0.43 (eV)	−0.09	0.07	0.08	—
Emery model	0.29 (t_{pd})	−0.11	0.05	−0.0056	−0.0003
This work	0.28 (t_{pd})	−0.136	0.068	0.061	−0.017

$$E_{2D}(k_x, k_y) = -2t\left[\cos(k_x a) + \cos(k_y a)\right] - 4t' \cos(k_x a)\cos(k_y a) - 2t''\left[\cos(2k_x a) + \cos(2k_y a)\right] - 4t'''\left[\cos(k_x a)\cos(2k_y a) + \cos(k_y a)\cos(2k_x a)\right]$$

Tight-binding model with nearby hoppings

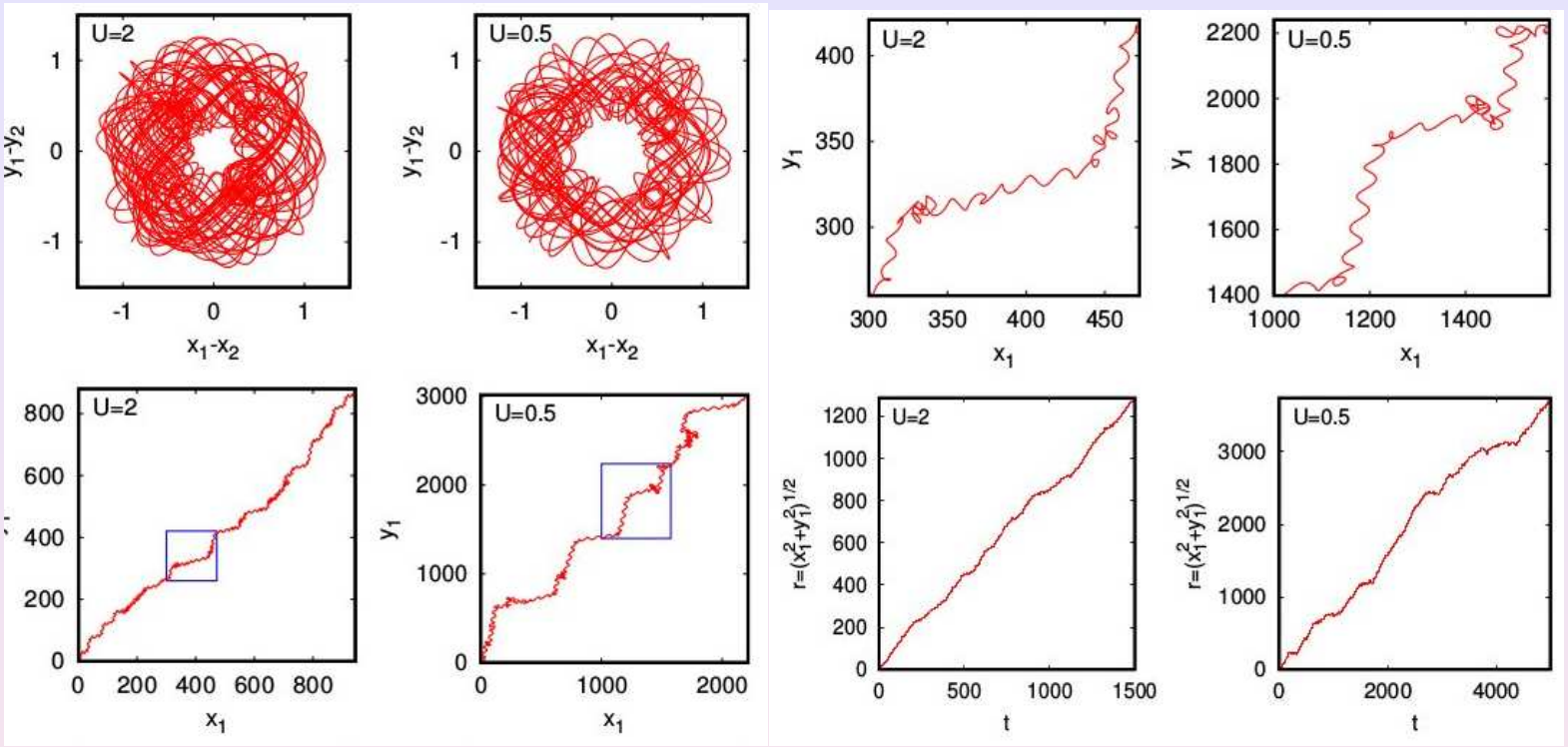
The quantum Hamiltonian of the model in $d = 1$ or 2 dimensions has the standard form [1–3]

$$H = -\sum_{\langle j,l \rangle} |j\rangle\langle l| + \sum_{j} \frac{U}{1 + r(j)} |j\rangle\langle j|, \qquad (1)$$

where $j = (x_1, x_2)$ $[j = (x_1, x_2, y_1, y_2)]$ is a multi-index for $d = 1$ $(d = 2)$; each index variable takes values $x_1, x_2, y_1, y_2 \in \{0, \ldots, N-1\}$, with N the linear system size with periodic boundary conditions. The first sum in (1) describes the electron hopping between nearby sites on a one-dimensional (1D) (or 2D square) lattice with a hopping amplitude taken as the energy unit. The second sum in (1) represents a (regularized) Coulomb-type long-range interaction with amplitude U and the distance $r(j)$ between two electrons. For one

When interaction is much larger than a noninteracting energy band there are pairs of two electrons propagating together due to pair energy conservation; but this case is not realistic (hopping $t = 1$, $U \gg B_d \approx 8d$).

Classical chaotic dynamics of electron pair



Classical Hamiltonian and chaos

The corresponding classical dynamics in two dimensions is described by the Hamiltonian

$$H = -2 \sum_{\mu=1,2;\alpha\in\{x,y\}} \cos p_{\mu\alpha} + U_C(x_1, x_2, y_1, y_2), \qquad (2)$$

with $U_C = U/[1 + \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}]$ and conjugated variables of momentum $p_{\mu x}$ and $p_{\mu y}$ and coordinates x_μ and y_μ [in one dimension we have in (2) only $p_{\mu x}$ and x_μ]. In one

Pairing mechanism at moderate Coulomb repulsion

Energy and momentum of pair ($p_{+x,y} = p_{1x,y} + p_{2x,y}$) are conserved

Writing $\cos(p_{1x}) + \cos(p_{2x}) = 2\cos(p_{+x}/2)\cos[(p_{2x} - p_{1x})/2]$ (and similarly for y), we see that at given values of p_{+x} and p_{+y} the kinetic energy is bounded by $\Delta E = 4\sum_\alpha |\cos(p_{+\alpha}/2)|$. Therefore, for TIP states with $E > \Delta E$, the two electrons cannot separate and they propagate as one pair. In particular, for $p_{+x} = p_{+y} = \pi + \delta$ (with $|\delta| \ll 1$) close to π, there are compact Coulomb electron pairs even for very small interactions U as soon as $\Delta E \approx 2d|\delta| < U \ll B_d$, with $B_d = 8d + U$ the maximal energy bandwidth in d dimensions. The center of mass velocity of such pairs [in direction $\alpha \in \{x, y\}$] is $v_{+\alpha} = (v_{1\alpha} + v_{2\alpha})/2 = 2\cos(\delta/2)\sin(p_{1\alpha} - \delta/2) \approx 2\sin p_{1\alpha}$ and it may be close to a maximal velocity $v_{+\alpha} = 2$. Figure S1 of

and there is an effective narrow energy band of width:
$\Delta E \approx 2d|\delta| < U \ll B_d$ for $p_+ = p_y + = \pi + \delta$.

Time evolution of 2 electrons on 2D-NxN lattice

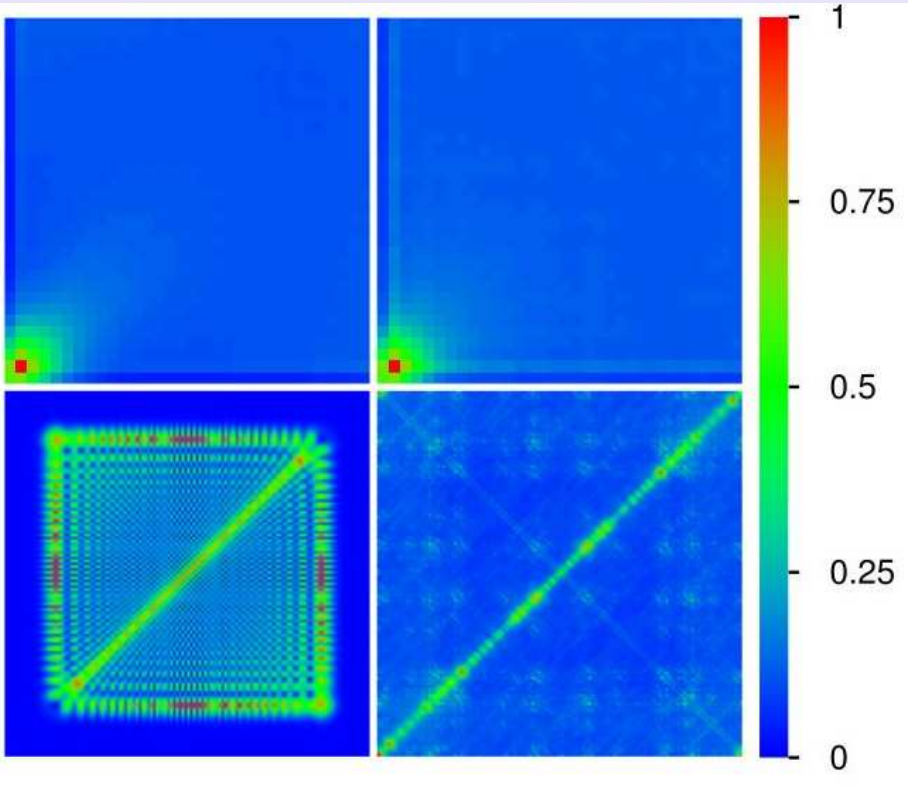


FIG. 3. Two-dimensional wave function densities obtained from the time evolution shown at times $t = 445\Delta t$ and $10^4\Delta t$ in left and right panels, respectively, for initial electron positions at approximately $(N/2, N/2)$, with $N = 128$ and $U = 2$ [$\Delta t = 1/B_2 = 1/(16 + U)$ is the Trotter integration time step]. The top panels show a close-up of the density for $(0 \leqslant \Delta x, \Delta y < 32)$ in the Δx-Δy plane of relative coordinates obtained from a sum over x_1 and y_1. The bottom panels show the density in the x_1-x_2 plane obtained from a sum over y_1 and y_2. The corresponding values of the probability near the diagonal w_{10} are $w_{10} = 0.106$ and 0.133 for the left and right

interaction $U = 2 \ll B_d = 16 + U$, Trotter integration time scheme
small size of pairs (a few lattice sites, like in La-based cuprates with a pair size of about 15*angstroms* (e.g. Dagotto Rev. Mod. Phys. (1994)

Eigenstates of 2 electrons on 2D-NxN lattice

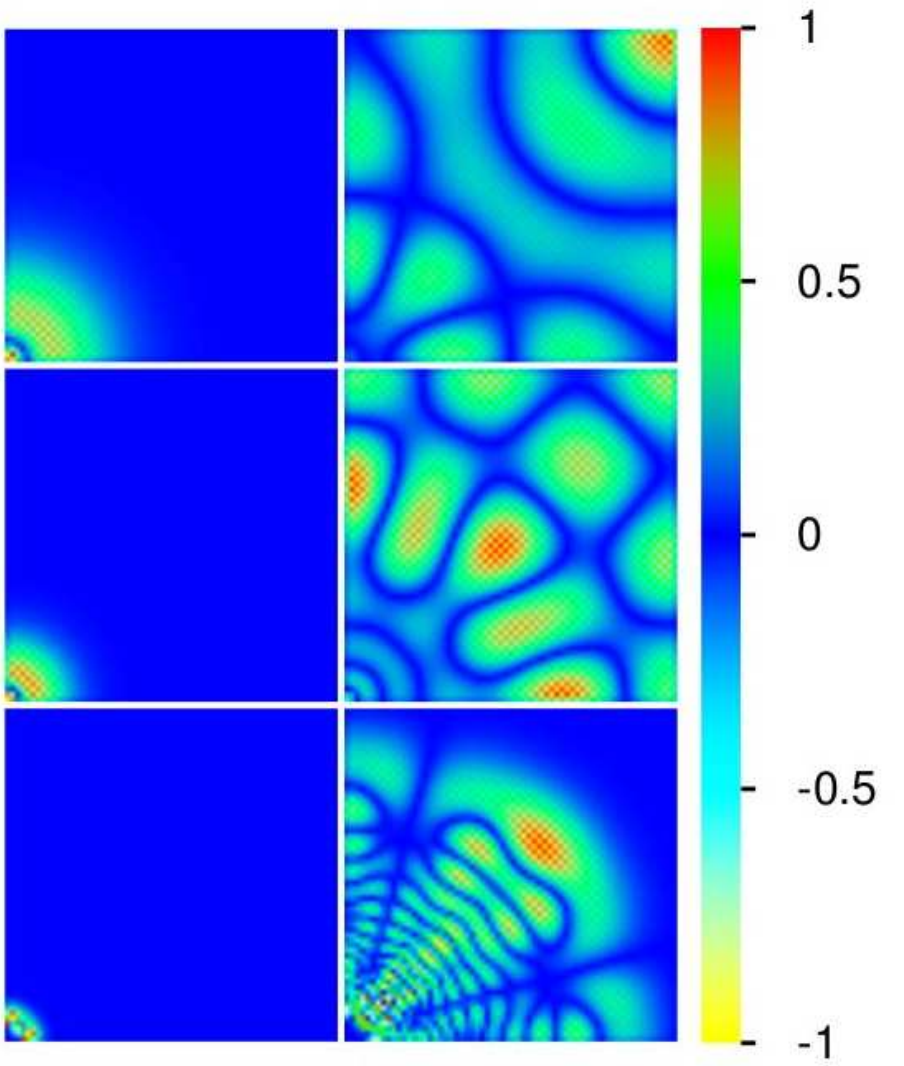


FIG. S7: Certain 2D (totally symmetrized) block eigenstates in Δx-Δy plane for $U = 2$, $N = 128$. Top panels correspond to conserved total momentum $p_+ = p_{+x} = p_{+y} = 0$ and block level numbers $l = 2143$ (left) and $l = 2135$ (right). Center panels correspond to $p_+ = 21\pi/32 \approx 2\pi/3$, $l = 2143$ (left), $l = 2131$ (right). Bottom panels correspond to $p_+ = 63\pi/64 \approx \pi$, $l = 2072$ (left), $l = 1991$ (right).

interaction $U = 2 \ll B_d = 16 + U; N = 128$

Time evolution on NxN and HTC lattices

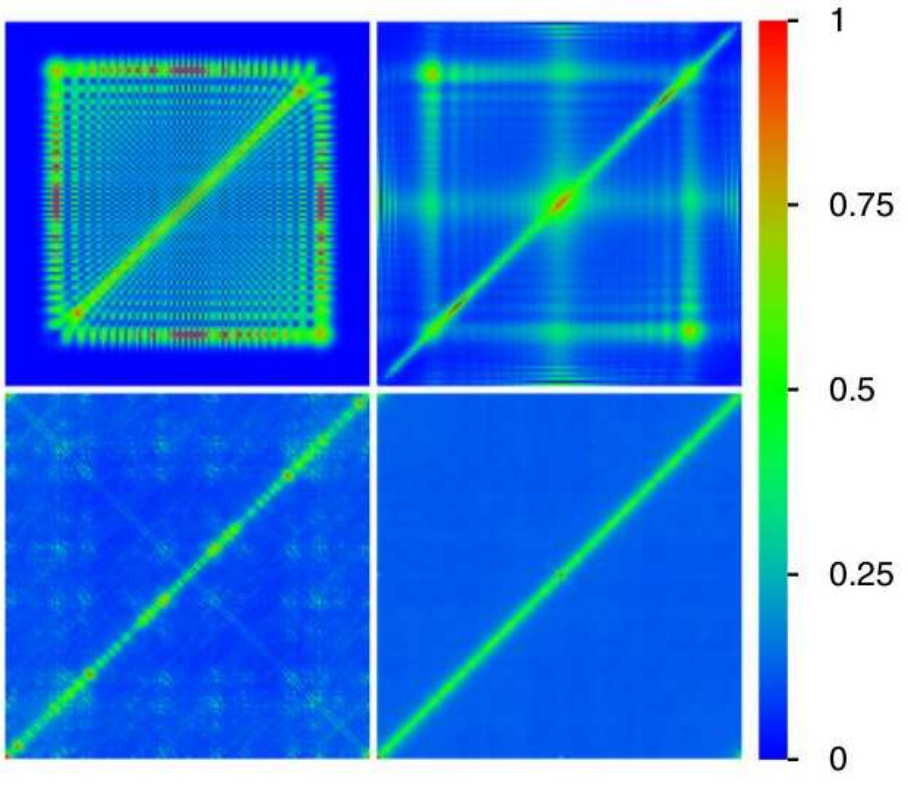


Fig. 2 2D Wavefunction density $\rho_{XX}(x_1, x_2)$ in x_1-x_2 plane (see Eq. (8)) obtained from the time evolution using the Trotter formula approximation for initial electron positions at $\approx (N/2, N/2)$ with distance $\Delta\bar{x} = \Delta\bar{y} = 1$ for $N = 128$, $U = 2$ and Trotter integration time step $\Delta t = 1/B_2 = 1/(16+U)$. Top (bottom) panels correspond to the time value $t = 445\,\Delta t$ ($t = 10^4 \Delta t$) and left (right) panels correspond to the NN-lattice (HTC-lattice). The corresponding values of the pair formation probability w_{10} are 0.106 (top left), 0.133 (bottom left), 0.0940 (top right) and 0.125 (bottom right). Related videos are available at [14,15]

interaction $U = 2 \ll B_d = 16 + U$; $N = 128$; NxN/HTC lattice left/right

Pair size on NxN and HTC lattices

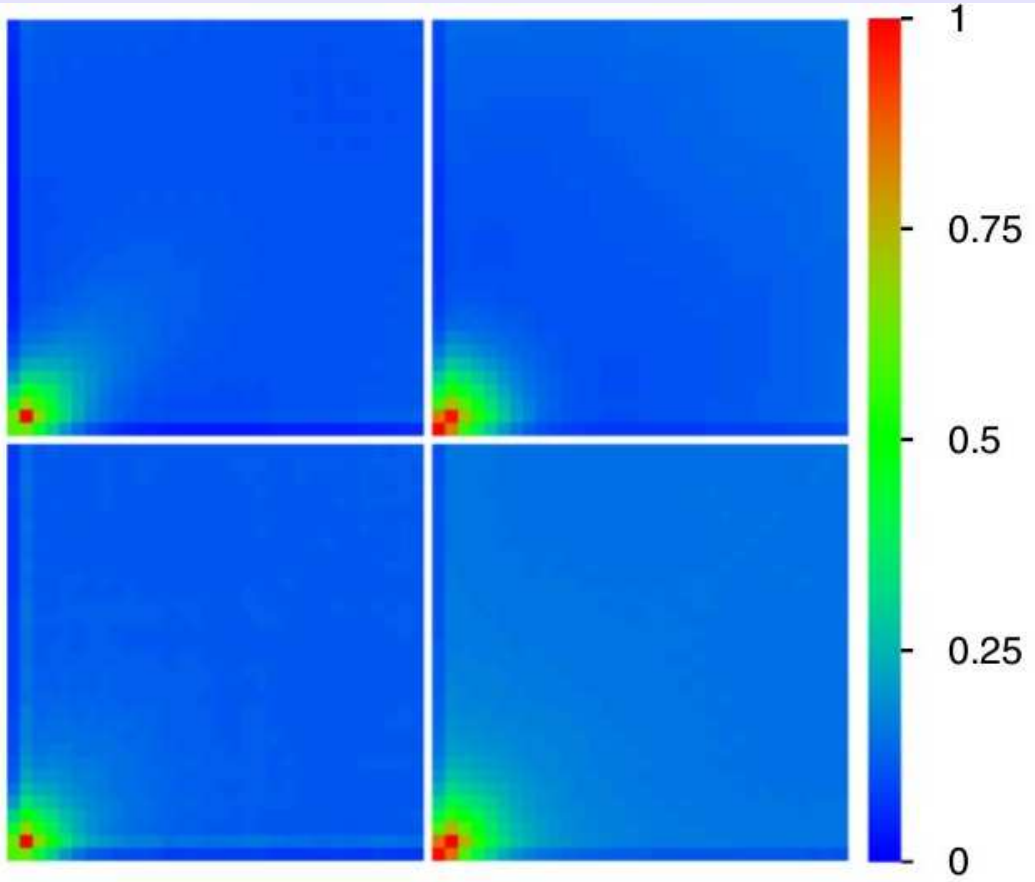


Fig. 3 2D Wavefunction density $\rho_{\rm rel}(\Delta x, \Delta y)$ in Δx-Δy plane of relative coordinates (see Eq. (9)) for the same states, cases and parameters of Fig. 2 ($N = 128$, $U = 2$). All panels show the zoomed density for $0 \leq \Delta x, \Delta y < 32$. Related videos are available at [14,15]

interaction $U = 2 \ll B_d = 16 + U$; $N = 128$; NxN/HTC lattice left/right; same parameters as on a previous slide

Probability of pair formation on NxN and HTC lattices

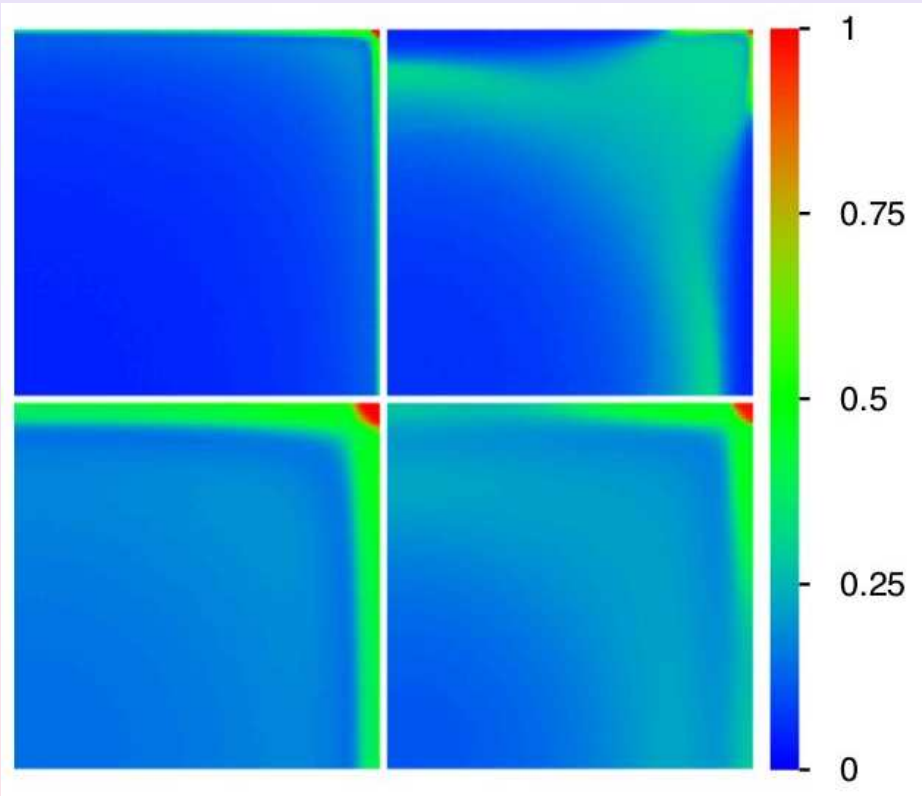


Fig. 4 Phase diagram of electron pair formation in the plane of pair momentum $\mathbf{p}_+ = (p_{+x}, p_{+y})$ for the NN-lattice (left panels), the HTC-lattice (right panels) and the interaction values $U = 0.5$ (top panels), $U = 2$ (bottom panels). Shown is the pair formation probability w_{10} for $N = 192$ obtained from the exact time evolution for each sector of $\mathbf{p}_+$ with an initial electron distance $\Delta\bar{x} = \Delta\bar{y} = 1$ and computed from an average over 21 time values in the interval $10^4 \leq t/\Delta t \leq 10^6$. In all panels the horizontal (vertical) axis corresponds to p_{+x} (p_{+y}) $\in [0, \pi]$ and the numerical values of the color bar correspond to the ratio of w_{10} over its maximal value. The maximum values corresponding to the red region at the top right corner $\mathbf{p}_+ = (\pi, \pi)$ are $w_{10} = 1$ (both left panels), $w_{10} = 0.4510$ (top right) and $w_{10} = 0.8542$ (bottom right). For comparison the ergodic value is $w_{10,\mathrm{erg.}} = (21/192)^2 = 0.01196$

color gives probability w_{10} of 2 electrons in a band distance 10 for NxN (left) and HTC (right) lattice

Probability of pair formation on HTC lattice

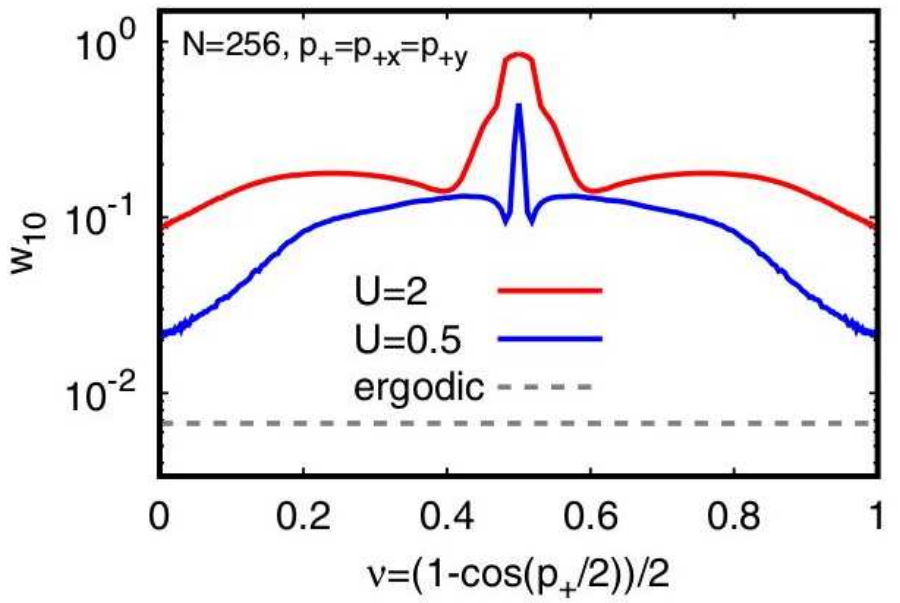


Fig. 6 Dependence of the electron pair formation probability w_{10} on $\nu = (1 - \cos(p_+/2))/2$ for $p_+ = p_{+x} = p_{+y}$ and the HTC-model at $U = 0.5, 2$ and $N = 256$. w_{10} is computed from the same long time average as in Fig. 4.

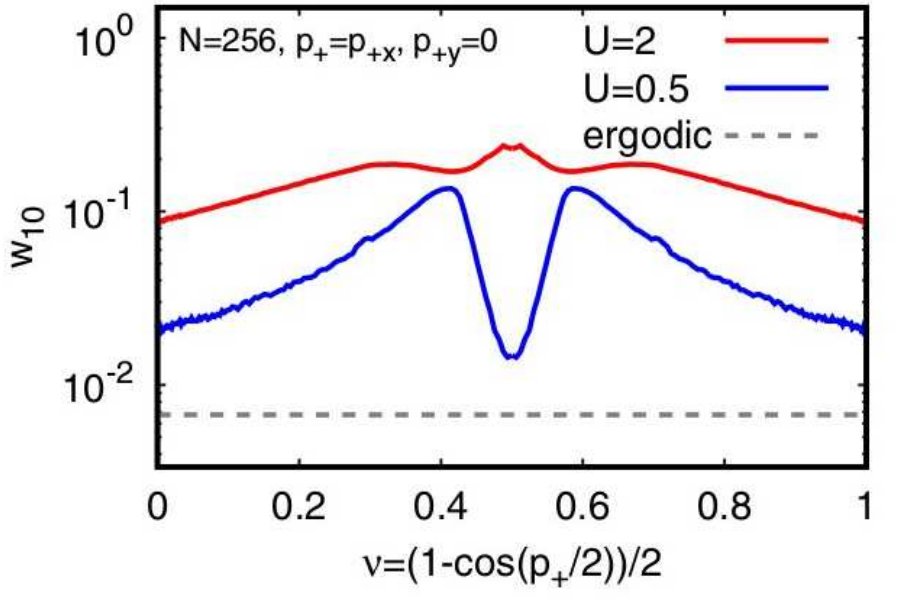


Fig. 7 Dependence of the electron pair formation probability w_{10} on $\nu = (1 - \cos(p_+/2))/2$ for $p_+ = p_{+x}, p_{+y} = 0$ and the HTC-model at $U = 0.5, 2$ and $N = 256$. w_{10} is computed from the same long time average as in Fig. 4.

Optimal probability of pair formation

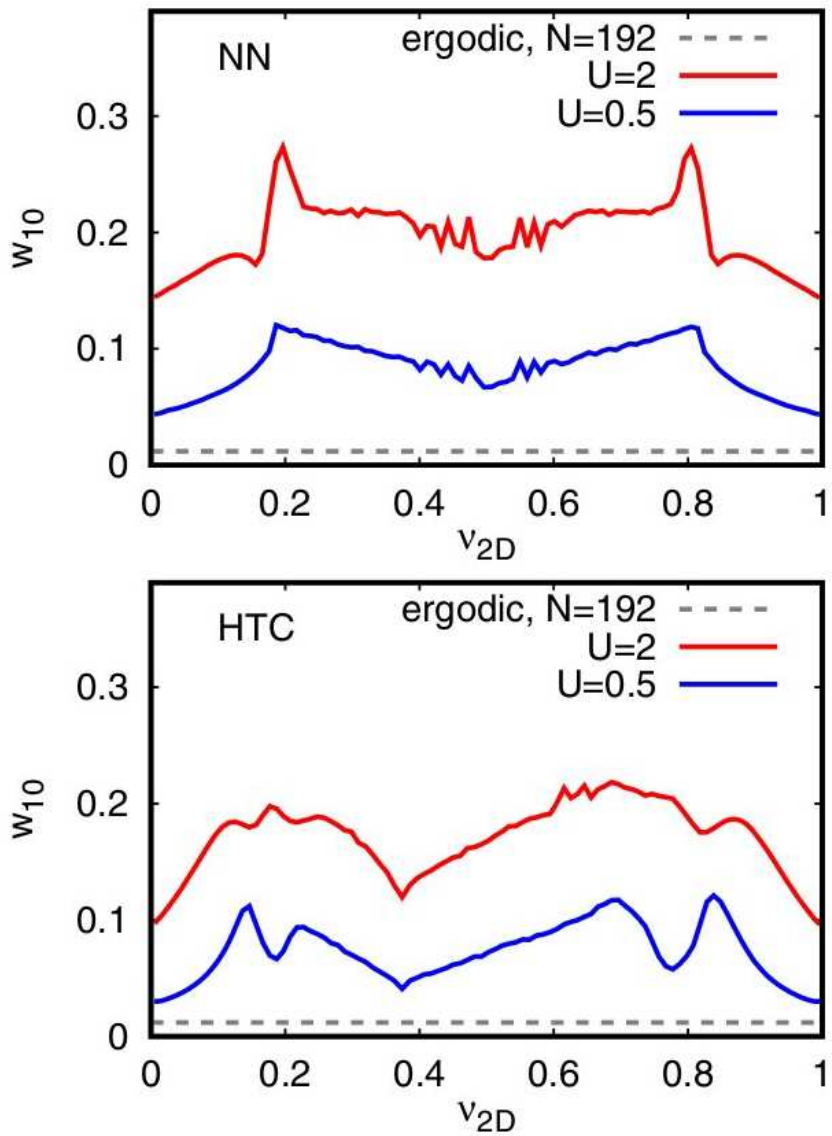


Fig. 10 Dependence of the electron pair formation probability w_{10} on the effective 2D filling factor ν_{2D} for the NN-lattice (top) and the HTC-lattice (bottom). The values of w_{10} have been obtained from the data of Fig. 4 (for $N = 192$) by an average along lines of constant electron pair energy E_c at momenta $\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}_+/2$ with $p_{+x}, p_{+y} \in [0, 2\pi]$. Lowest (largest) energy corresponds to $\nu_{2D} = 0$ ($\nu_{2D} = 1$). The data points shown correspond to an effective histogram with bin width $\Delta\nu_{2D} \approx 0.01$. The red (blue) curve corresponds to the interaction value $U = 2$ ($U = 0.5$) and the grey dashed line corresponds to the ergodic value $(21/192)^2 = 0.01196$

optimal $\nu_{2D} \approx 0.2(0.8)$ for NxN and $\nu_{2D} \approx 0.2(0.75)$ depending on U for HTC lattice

Discussion

* Formation of two-electron pairs by moderate Coulomb repulsion in band structures
* Relatively small size of pairs being of about 3-10 lattice spacings
* Maximal probability of pair formation at filing factor $\nu_{2D} \approx 0.2(0.8)$
* Problem remaining: finite electron density case; ihomogeneous electron density at low energys and pairs near Fermi energy?