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Phys. Rev. B **94**, 214501 — Published 1 December 2016

DOI: 10.1103/PhysRevB.94.214501

Superconductivity in repulsively interacting fermions on a diamond chain: flat-band induced pairing

Keita Kobayashi,[1] Masahiko Okumura,[1] Susumu Yamada,[1,2] Masahiko Machida,[1] and Hideo Aoki[3,4]

[1]*CCSE, Japan Atomic Energy Agency, Kashiwa, Chiba 277-0871, Japan*
[2]*Computational Materials Science Research Team, RIKEN AICS, Kobe, Hyogo 650-0047, Japan*
[3]*Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan*
[4]*Electronics and Photonics Research Institute, Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan*

(Dated: October 24, 2016)

To explore whether a flat-band system can accommodate superconductivity, we consider repulsively interacting fermions on the diamond chain, a simplest quasi-one-dimensional system that contains a flat band. Exact diagonalization and the density-matrix renormalization group (DMRG) are used to show that we have a significant binding energy of a Cooper pair with a long-tailed pair-pair correlation in real space when the total band filling is slightly below 1/3, where a filled dispersive band interacts with the flat band that is empty but close to E_F. Pairs selectively formed across the outer sites of the diamond chain are responsible for the pairing correlation. At exactly 1/3-filling an insulating phase emerges, where the entanglement spectrum indicates the particles on the outer sites are highly entangled and topological. These come from a peculiarity of the flat band in which "Wannier orbits" are not orthogonalizable.

PACS numbers: 74.20.Rp, 71.10.Fd, 67.85.Lm

Introduction— While fascinations with unconventional superconductivity arising from electron correlation continue to increase, as exemplified by the high-T_C cuprates and iron-based superconductors, a next question to ask is whether there exists an avenue where we have superconductivity with another pairing mechanism. Namely, in the superconductivity in correlated electron systems, the standard viewpoint is that the interaction mediated by spin fluctuations glues the electrons into anisotropic pairs such as d-wave or s_{+-}, where the nesting of the Fermi surface dominates the fluctuation, hence the superconductivity. To look for a different class of models, one intriguing direction is to consider correlated systems on flat-band lattices that contain dispersionless band(s) in their band structure. This is because, regardless of the Fermi energy residing on or off the flat band, we cannot define the Fermi surface for the flat band. In other words, we cannot apply, in one-dimensional cases, Tomonaga-Luttinger picture for the states around E_F even with multichannel g-ology unlike the case of ladders. Thus, if superconductivity does arise, this might harbor a mechanism in which the flat band plays a role distinct from the conventional, nesting-dominated boson-exchange mechanisms.

In the field of ferromagnetism, on the other hand, there is a long history for the study of flat-band ferromagnetism[1–3], which is distinct from the conventional (Stoner) ferromagnetism. The ferromagnetic ground state is rigorously shown for arbitrary repulsive interaction $0 < U \leq \infty$ when the flat band is half-filled. The flat-band lattice models are conceived as Lieb model[1] with different numbers of A and B sublattice sites, or Mielke and Tasaki models[2,3] such as kagome lattice. A speciality of these flat-band lattices appears as an anomalous situation that Wannier orbitals cannot be orthogonalized, which is called the connectivity condition for the density matrix[4]. This immediately dictates that the flat band arises from interferences, hence totally different from the atomic (zero-hopping) limit, and indeed the flat-band models are necessarily multi-band systems, where the flat band(s) coexist with dispersive ones. Flat-band systems are not merely a theoretical curiosity, but candidate systems have been considered[5]. Also, recent developments in cold-atom Fermi gases on optical lattices are a promising arena, where Lieb[6] and kagome[7] lattices are already discussed.

Thus the flat-band system provides a unique playground, because the correlation effects should be strong for the flat bands (as briefly described in Supplementary Material C), but also because of the above-mentioned unusual structure of the density matrix (or strongly interfering wave functions). We can thus envisage dramatic, possibly non-perturbative phenomena from the electron-electron interaction on these macroscopically degenerate manifolds of single-particle states. Beside the ferromagnetism, the flat band systems have attracted recent attentions for possible realization of topological insulators with non-trivial Chern numbers[8–12]. The next goal, in our view, is to realize superconductivity in flat-band systems. We shall show here that there are indeed signatures for pairing for repulsively interaction electrons in a one-dimensional flat-band lattice.

Theoretically, exploration of superconducting phases in flat-band systems is quite challenging, since correlation effects become even more difficult to fathom for the flat bands than in ordinary ones[13]. Thus far, possibility of pair formation on flat bands has been examined by several authors. Pairing of two fermions on diamond chain with π-flux inserted was discussed by Vidal *et al.*[14] Kuroki *et al.* have considered a cross-linked ladder that contains wide and narrow (or flat) bands in the context of the high-T_C cuprate ladder compound,[15] and have shown that superconducting T_C estimated from the fluctuation exchange approximation (FLEX) is much higher than in usual lattices when E_F is just above the flat band that interspears the dispersive one. There, virtual pair scatterings between the dispersive and fully-filled flat bands are suggested to cause the high T_C. Pair formation has also been discussed for bose Hubbard model on cross-linked ladders,[16,17] where a large pair hopping gives rise to the emergence of a superfluid phase (pair Tomonaga-Luttinger liquid) overlapping with a Wigner-solid region in the phase diagram. Namely, in flat-band systems, not only pair hopping amplitudes can be large, but also diagonal orders tend to coexist (rather than compete) with superfluids. These results suggest that the flat bands may be indeed a good place to look for pair condensates.

This has motivated us here to explore superconductivity for a repulsive fermionic Hubbard model on flat band systems. As a model we take a simplest possible, quasi-1D lattice comprising a chain of diamonds as depicted in Fig.1(a). We shall show that for E_F close to but slightly below the flat band (with the filling of the whole bands slightly below 1/3), attractive binding energies appear. Concomitantly, the pair-pair correlation becomes long-tailed in real space at these band fillings.

Model and methods — As methods for calculation we opt for exact diagonalization and the density-matrix renormalization group (DMRG) that can deal with strong correlation, since the correlation phenomena on flat bands may well call for such non-perturbative methods. For the position of the Fermi energy, E_F, we focus on the regime where the flat band is empty. This choice comes from the following observation. When the flat band is half filled, the ground state is ferromagnetic. When E_F is shifted but still on the flat band, the diverging density of one-electron states is expected to give rise to large self-energy corrections, which should be detrimental to superconductivity. When the flat band is empty with E_F residing in a dispersive band, this problem can be resolved, with virtual processes between the dispersive and flat bands still at work. For bipartite lattices such as the diamond chain, the empty flat band is equivalent to fully-filled flat band due to an electron-hole symmetry

It is desirable to have, on top of E_F, another control parameter about the flat band. So here we introduce a hopping t' between the adjacent apex sites of diamonds (Fig.1(a)). For $t'=0$ the lattice (a Lieb model) is bipartite with the flat band as a middle one in this three-band system. As we increase t' the bands are deformed, until in the limit $t'/t=1$ the bottom band becomes flat (a Mielke model). Thus we can examine how the pairing behaves as we change $t'=0\to 1$. We then calculate the binding energy of pairs with the exact diagonalization (ED), and pair-pair (and other) correlation functions with the DMRG[18–21].

We take the conventional Hubbard Hamiltonian on the diamond chain (Fig.1(a)),

$$H = H_{\rm kin} + H_{\rm int}\,, \tag{1}$$

$$H_{\rm kin} = t\sum_{i,\sigma=\uparrow\downarrow} c^\dagger_{2,i,\sigma}\sum_{m=1,3}(c_{m,i,\sigma}+c_{m,i+1,\sigma}) + t'\sum_{i,\sigma=\uparrow\downarrow}\sum_{m=1,3} c^\dagger_{m,i,\sigma}c_{m,i+1,\sigma} + {\rm h.c}\,, \tag{2}$$

$$H_{\rm int} = U\sum_{m,i} n_{m,i,\uparrow}n_{m,i,\downarrow}\,, \tag{3}$$

where t (unit of energy) and t' are the nearest-neighbor and inter-apex hoppings, respectively, $c^\dagger_{m,i,\sigma}$ creates a fermion with spin σ on the m-th leg at the i-th unit cell, $n_{m,i,\sigma} = c^\dagger_{m,i,\sigma}c_{m,i,\sigma}$, and $U>0$ is the on-site repulsive interaction. Figure 1(b) shows the band structure, $\epsilon(k) = \pm[4(1+\cos(k))+(t')^2\cos^2(k)]^{1/2}+t'\cos(k)\,, 2t'\cos(k)$, in the noninteracting case ($U=0$). As we can see, one of the three bands becomes flat in the limit of $t'=0$ or 1. We focus on the region where the filling of the whole bands is around 1/3 (one fermion per unit cell on average) to investigate the effects of repulsive interaction. We have, for $t'=0\to 1$, a fully-occupied bottom band which touches the middle band at $k=\pm\pi$, where the middle (bottom) band becomes flat at $t'=0$ (1).

Intriguingly, we have noticed in performing the DMRG that we have to keep an unusually large number of states up to $m_{\rm DMRG}=1500$ for the present ladder-like lattice. For DMRG we take an open boundary condition with inversion-symmetric configurations as shown in Fig.1(a). Here we focus on the properties below 1/3-filling to explore the possibility of fermion superfluidity in terms of the pair binding energy and correlation functions.

Results— Let us first examine the fermion pair formation in terms of the binding energy, $\Delta E_b \equiv E_g(N_\uparrow+1,N_\downarrow+1)+E_g(N_\uparrow,N_\downarrow)-2E_g(N_\uparrow+1,N_\downarrow)$, where $E_g(N_\uparrow,N_\downarrow)$ is the ground-state energy for $N_{\rm tot}=N_\uparrow+N_\downarrow$ fermions with N_σ being the total number of σ-spin electrons. A negative ΔE_b implies that an attractive interaction works between two particles. $E_g(N_\uparrow,N_\downarrow)$ is computed with ED in periodic boundary conditions. In the numerical calculation, we set the total number of sites to be $N=18$ with the length of the chain being $L=N/3=6$.

Figure 2(a) shows ΔE_b as a function of the filling $n=N_{\rm tot}/2N$ for $t'=0$ for various values of U/t. We can immediately notice that two electrons become bound (i.e., ΔE_b becomes negative) sharply around $n=1/3$ ($N_\uparrow=N_\downarrow=6\,, N=18$) for all the values of $U>0$ considered. Interestingly, the binding energy is not monotonic against U but peaked around $U/t=4$. As we shall see, the binding occurs for two electrons sitting on the $m=1$ and 3-legs. The binding energy continues to be negative just below $n=1/3$. In the other flat-band limit at $t'/t=1$, we can see in Fig.2(b) that we have again a binding at a filling slightly smaller than 1/3 (5/18-filling), where ΔE_b becomes negative.

We now proceed to DMRG calculations for various correlation functions, including pair correlation, on the diamond chain[23]. The density (D_m) and spin (S_m) correlation functions on the m-th leg are defined respectively as

$$D_m(i,j) = \langle n_{m,i} n_{m,j} \rangle - \langle n_{m,i} \rangle \langle n_{m,i} \rangle \,, \quad (4)$$

$$S_m(i,j) = \langle S^{(z)}_{m,i} S^{(z)}_{m,j} \rangle \,, \quad (5)$$

with $n_{m,i} = n_{m,i,\uparrow} + n_{m,i,\downarrow}$ and $S^{(z)}_{m,i} = (n_{m,i,\uparrow} - n_{m,i,\downarrow})/2$. We compute the correlation functions on leg $m = 1$ and on 2 (while the correlation functions on $m = 3$ is equivalent to those on $m = 1$). The singlet-pair correlation functions are defined as

$$C^{\rm pair}_{\{m'm\}}(i,j) = \langle \Delta_{m'm,j} \Delta^{\dagger}_{m'm,i} \rangle \,, \quad (6)$$

$$\Delta_{m'm,i} \equiv c_{m',i+l,\uparrow} c_{m,i,\downarrow} - c_{m',i+l,\downarrow} c_{m,i,\uparrow} \,, \quad (7)$$

where l characterizes the pair [see Fig.3(a)].

The result for various correlations in Fig.3(b) reveals that the dominant (most long-tailed with distance r) correlation for $U/t \neq 0$ in the vicinity of 1/3-filling ($n \simeq 0.329$ with $N_{\uparrow} = N_{\uparrow} = 54$ and $N = 164$) is the pair correlation $|C^{\rm pair}_{\{31\}}(r)|$ for the pair,

$$\Delta_{31,i} = c_{3,i,\uparrow} c_{1,i,\downarrow} - c_{3,i,\downarrow} c_{1,i,\uparrow},$$

across $m = 1$ and 3 (see Fig.3(a)).[22] The next dominant correlations are the pair $C^{\rm pair}_{\{11\}}(r)$ (for $\Delta_{11,i} = c_{1,i+1,\uparrow} c_{1,i,\downarrow} - c_{1,i+1,\downarrow} c_{1,i,\uparrow}$) and density $D_1(r)$ correlations on $m = 1$. Then comes the spin $S_1(r)$ correlation on $m = 1$. On the other hand, the correlations on $m = 2$ (see $C^{\rm pair}_{\{21\}}(r)$ and Supplementary Material B) rapidly decay for all the values of n studied here[23]. As in the density and spin correlations, the pair correlation involving $m = 2$ ($\Delta_{21,i} = c_{2,i,\uparrow} c_{1,i,\downarrow} - c_{2,i,\downarrow} c_{1,i,\uparrow}$) shows a fast decay. The dominant $\Delta_{31,i}$ is consistent with an analysis of the entanglement entropy and edge states at $t' = 0$ in Supplementary Material A.

The reason why all of the pair, density and spin correlations develop on legs $m = 1, 3$ in the vicinity of 1/3-filling can be considered as coming from the basis functions on the flat band. When the hopping t' is absent, we can introduce a basis,

$$\alpha_{i,\sigma} = c_{2,i,\sigma} \,, \quad \beta_{i,\sigma} = (c_{1,i,\sigma} + c_{3,i,\sigma})/\sqrt{2} \,,$$
$$\gamma_{i,\sigma} = (c_{1,i,\sigma} - c_{3,i,\sigma})/\sqrt{2} \,, \quad (8)$$

with which the kinetic part of Eq.(1) can be expressed as $H_{{\rm kin},t'=0} = \sqrt{2}t \sum_{i,\sigma} \alpha^{\dagger}_{i,\sigma}(\beta_{i,\sigma} + \beta_{i-1,\sigma}) + {\rm h.c}$. The basis $\{\gamma_{i,\sigma}\}$ represents the particles on the flat band (see left panel of Fig.1(c)), in which the probability amplitude selectively resides on legs $m = 1$ and 3 (i.e. on A sublattice if we divide the bipartite lattice). The interaction U then brings about interband matrix elements between the flat and dispersive bands around 1/3-filling. The development of superconductivity when the flat band is empty (which is equivalent to full filling in the present electron-hole symmetric lattice) is consistent with the result in Ref.[15]. While the latter uses FLEX, a weak-coupling method, the present result reveals the flat-band superconductivity is in fact prominent in a strong-coupling ($U/t \simeq 4$) regime. The behavior of the correlation functions enhanced on $m = 1, 3$ should come from the virtual states that have probability amplitudes residing on legs $m = 1$ and 3 with the long-range nature of the correlations involving orbits for the flat band.

What happens when the filling is exactly 1/3 is also interesting, so that we have studied the quantum phases at that filling in Supplemental Material A. Topological states are shown to emerge, which is indicated from the entanglement spectrum for spins on the outer sites as well as from emerging edge states. This is considered to be another effect of the unusual Wannier states in the flat band, and the pairing states for the E_F close to but away from the flat band seems to sits adjacent to a topological phase at the point where the flat band just becomes empty.

Summary— We have investigated repulsively interacting fermions on the diamond chain, a simplest possible quasi-1D flat-band system, with ED and DMRG calculations. The numerical results have revealed that when the band filling is slightly below 1/3 with the flat band close to but away from E_F, the pair binding energy calculated with ED has two sharp peaks at two flat-band limits ($t' = 0$ or 1). Then the DMRG shows that, for $t' = 0$, the most dominant correlation is the singlet-pair across the outer sites ($m = 1, 3$) of the diamond. For $t'/t = 1$, by constrast, a phase separated behavior is observed as indicated in Supplementary Material B. The flat band promoting superconductivity through virtual pair hoppings involving the band as conceived in FLEX[15] is shown to be prominent in a strong-coupling regime. It is an interesting future problem to see whether a mechanism beyond the boson-exchange is at work here, which will require methods that take account of vertex corrections.

While we have concentrated on the quasi-1D diamond chain, enhanced pairing correlations with the major component residing on the flat-band wave functions are expected to be a general property of the flat-band systems satisfying the connectivity condition. Extension of the present study to flat-band systems with fluxes inserted[14,16,25] is also an interesting future work. While the diamond-chain structure has been discussed for condensed-matter systems such as an insulating magnet azurite[26,27], cold atoms on optical lattices should be an ideal test bench for experimental realizations of flat-band lattices.

Acknowledgments

HA was supported by a JSPS KAKENHI (No. 26247057) and ImPACT project (No. 2015-PM12-05-01) from JST. SY and MM were partially supported by JSPS KAKENHI (Nos. 15K00178, 26400322, and 16H02450).

The numerical work was in part performed on Fujitsu BX900 at JAEA.

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Figures

FIG. 1: (Color Online) (a) Hubbard model on a diamond chain with t (t') the nearest-neighbor (inter-apex) hoppings, m labeling the leg while i the unit cell. Also shown are two types of cuts (vertical and diagonal), which are used in DMRG calculation of the entanglement entropy. (b) Band structures in the noninteracting case ($U = 0$) for various values of t', with shaded areas indicating the 1/3 filling. (c) Orbits considered here for the flat band at $t'/t = 0$ or 1.

FIG. 2: (Color Online) (a,b) ED result for the binding energy $\Delta E_{\rm b}$ vs band filling n for $t' = 0$ (a) or $t'/t = 1$ (b) for various values of U/t with $N = 18$ sites here. (c,d) Binding energy $\Delta E_{\rm b}$ vs t'/t for band filling $n = 5/18$ (c) or $n = 1/3$ (d) for various values of U/t. Top panel is a color-code plot of $\Delta E_{\rm b}$ against n and t'/t for $U/t = 4$, where arrows indicate the cross sections displayed in panels (a-d).

FIG. 3: (Color Online) (a) Correlation of various possible pair configurations on the diamond chain with $t' = 0$. (b) Absolute values of various pair correlation functions are shown against real-space distance r along with density and spin correlation functions for $U/t = 4, n = 0.329$. (c) Pair correlation $C^{\rm pair}_{\{31\}}(r)$ against r for various values of n for $U/t = 4$. (d) Pair correlation $C^{\rm pair}_{\{31\}}(r)$ for various values of U/t for $n = 0.329$. Here the length of the chain is $L = 55$ (with 164 sites in total).

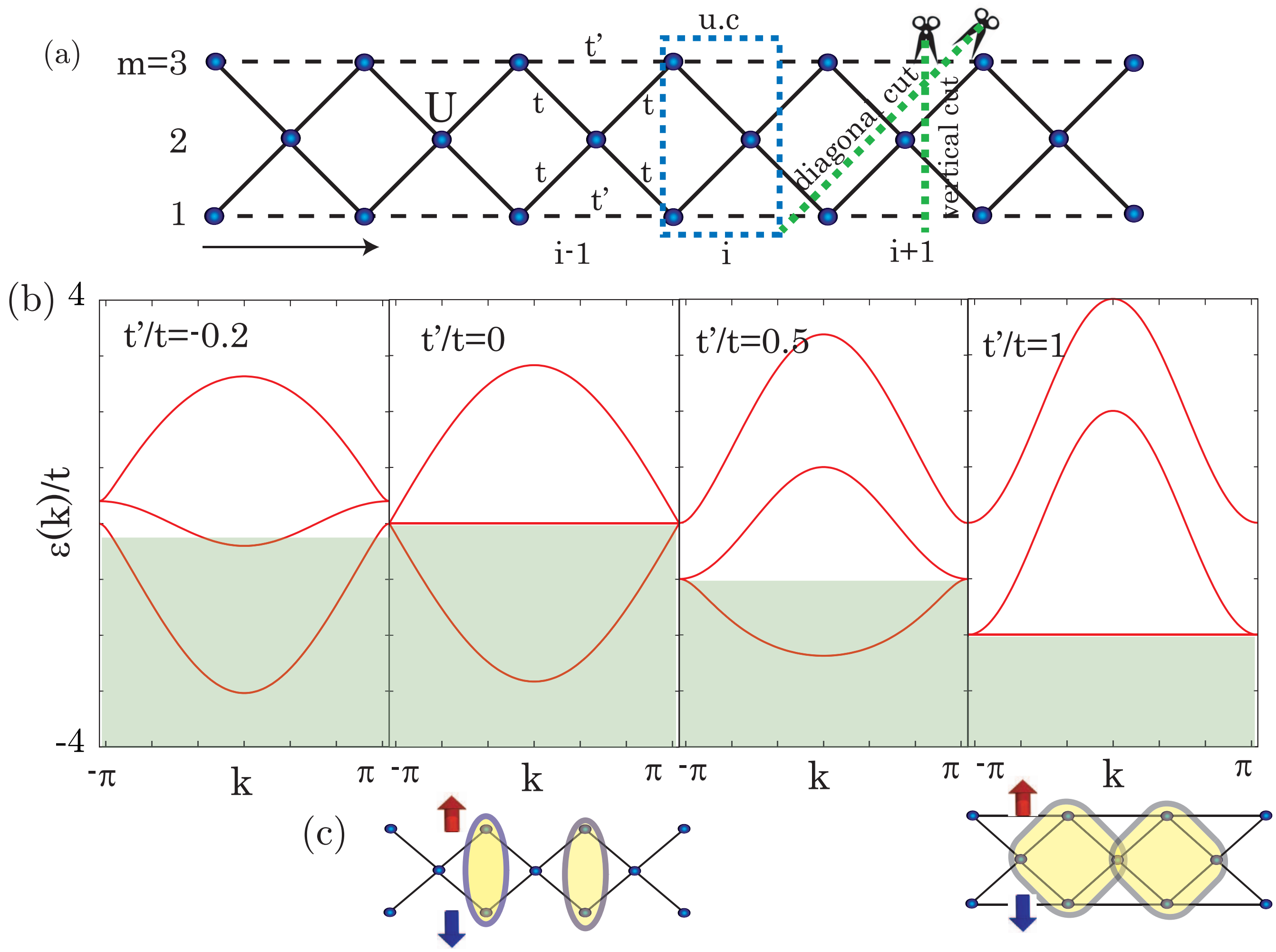

Figure 1 23OCT16

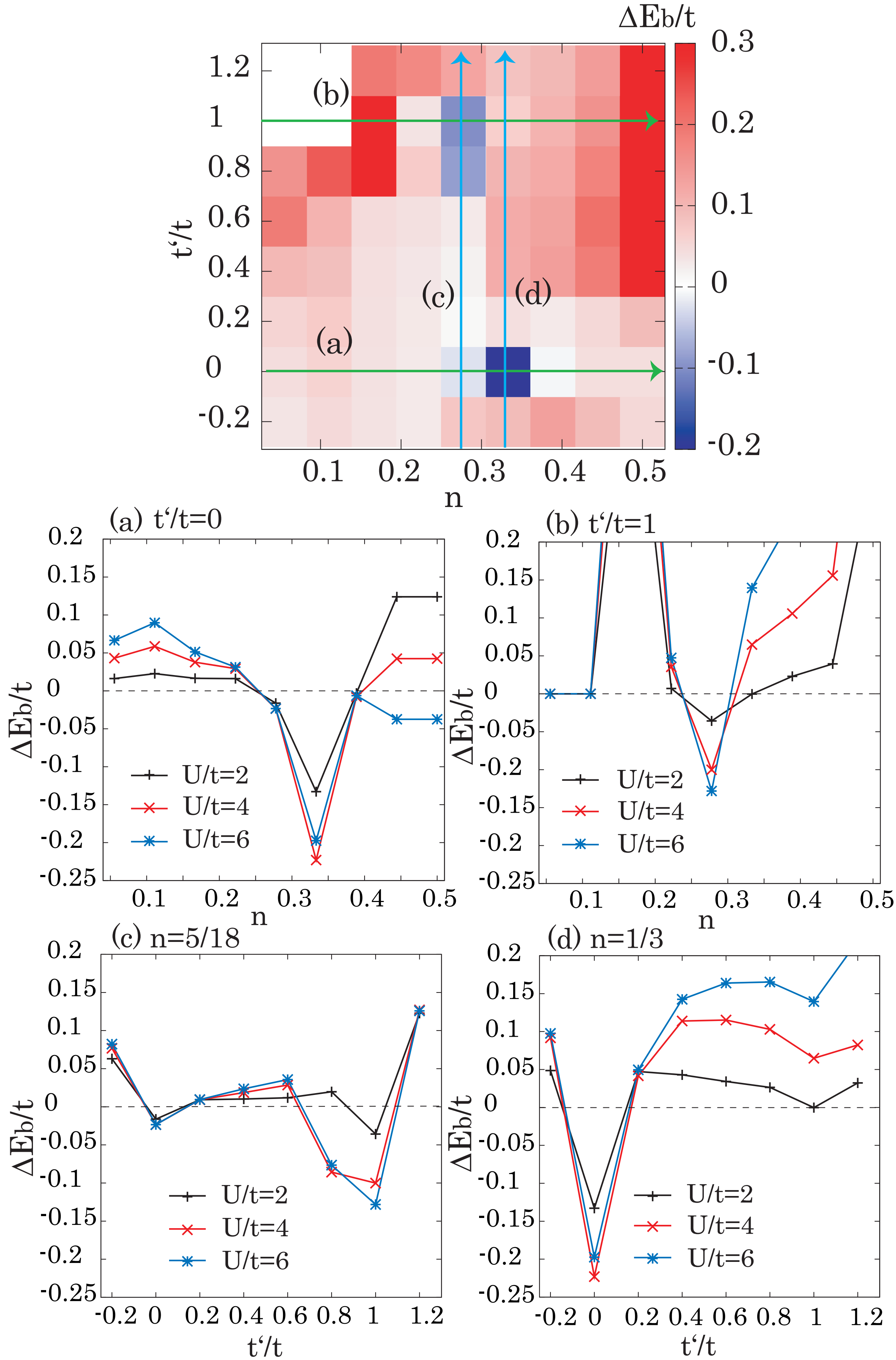

Figure 2 23OCT16

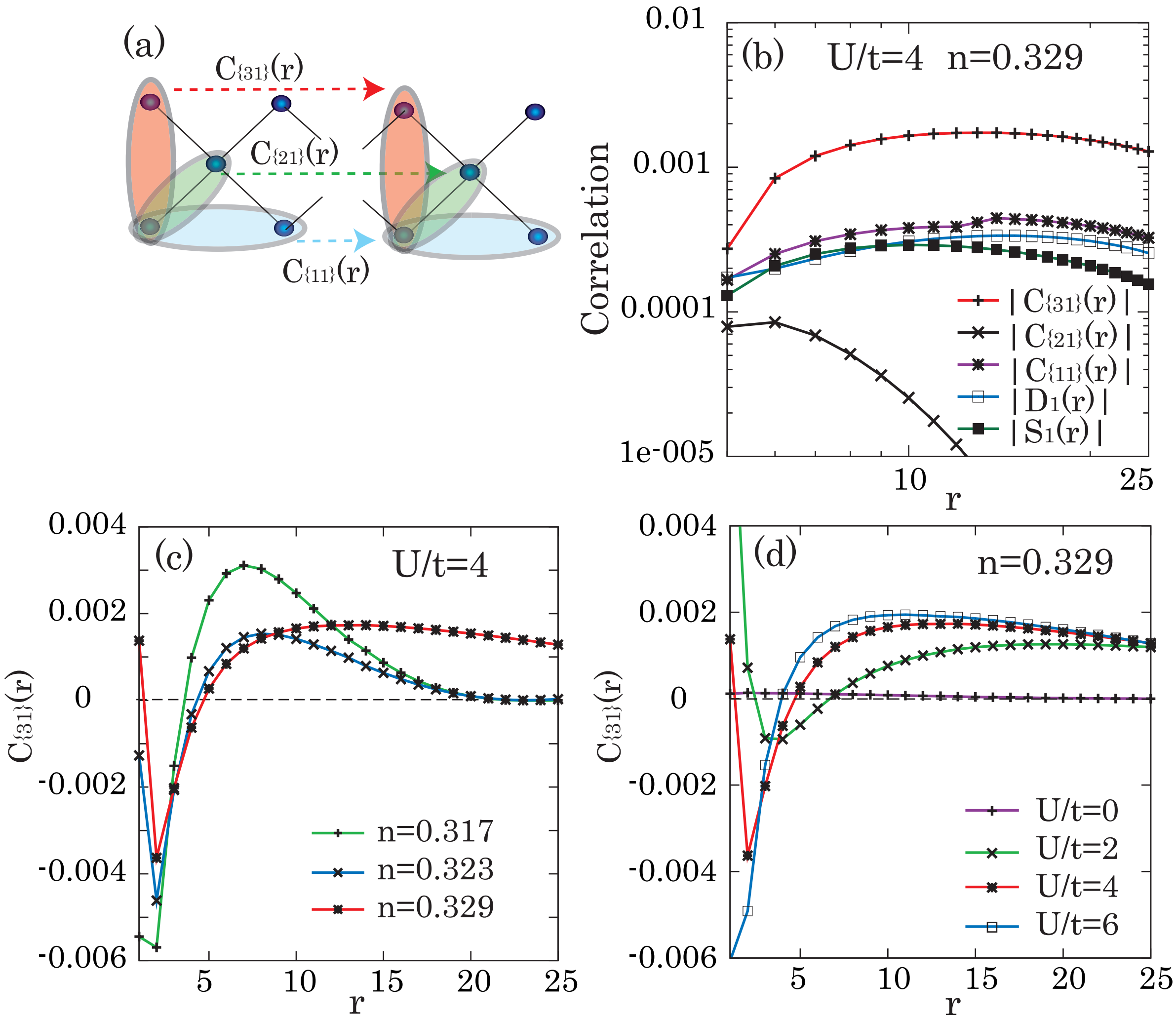

Figure 3 23OCT16