Few-body clusters in a multiband Hubbard model: tetramers, pentamers, and beyond

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We start with a variational approach and derive a set of coupled integral equations for the exact solutions of the bound states of \( N \) identical spin-up fermions and a single spin-down fermion in a generic multiband Hubbard Hamiltonian with onsite attractive interactions. As an illustration we apply the integral equations to the so-called sawtooth lattice up to \( N = 3 \), i.e., to the \((3 + 1)\)-body problem, due in part to its flat one-body band and one-dimensional simplicity, and most importantly to our benchmarking capacity with the DMRG simulations and exact diagonalization. Our numerical results reveal not only the presence of tetramer states in this two-band model but also their quasi-flat dispersion when formed in a flat one-body band. For \( N = \{4, 5, \cdots, 10\} \) our DMRG simulations and exact diagonalization suggest the presence of larger and larger multimers with lower and lower binding energies, conceivably without an upper bound on \( N \) and with a quasi-flat dispersion when formed in a flat one-body band. These peculiar \((N + 1)\)-body clusters are in sharp contrast with the exact results on the single-band linear-chain model where none of the \( N \geq 2 \) multimers appear.

Introduction: Exactly solvable few-body problems may offer valuable insights into the formation of complex many-body phenomena starting from a collection of isolated particles, dimers, trimers, and other multimers \([1–6]\). For instance the instability of a non-interacting Fermi gas against the formation of a Cooper pair on its top is a prime example, which eventually lead the way to the theory of BCS superconductivity. Up until very recently all of the few-body studies were focused either on continuum systems or on their lattice counterparts that feature a single band. In particular, followed by the experimental realization of the long-sought Efimov effect with ultracold bosons \([7–11]\), where three identical bosonic atoms that are interacting via short-range resonant interactions in vacuum exhibit an infinite series of three-body bound states, we have seen a growing interest in related effects with fermions. For instance three-body, four-body and and five-body Efimov effects have all been predicted, respectively, with two, three and four identical heavy fermions that are interacting resonantly with a much lighter particle \([12–19]\). Thus, as opposed to the equal-mass case where only dimer states are allowed, the multimer (trimer, tetramer and pentamer) states appear in mass-imbalanced mixtures when the mass-ratio exceeds a certain threshold depending on the multimer type. See recent reviews for a comprehensive list of related works \([1–5]\). Analogous predictions were also reported for the appearance of trimer states in single-band lattices only when the tunneling amplitudes are spin dependent \([20–24]\).

Despite all these progress it is surprising that the fate of multimers is still an uncharted territory when there exists more than one Bloch band in the one-body spectrum. For instance, in sharp contrast with the exact results on the single-band linear-chain model which dismiss all of the multimers \([6, 20, 21, 25]\), the energetic stability of the trimers have recently been predicted in a sawtooth lattice \([26, 27]\). In addition these trimers have a quasi-flat dispersion (with a negligible bandwidth) when formed in a flat band \([27]\), which is unlike the highly-dispersive spectrum of its dimers \([26, 27]\). Motivated by the success of variational approach on the two-body and three-body problems \([27–29]\), here we generalize it to the bound states of \( N \) identical spin-up fermions and a single spin-down fermion in a generic multiband Hubbard model with onsite attractive interactions. As an illustration we apply our \( N = 3 \) theory to the sawtooth lattice, and reveal both the energetic stability of the tetramer states in a two-band lattice and their quasi-flat dispersion when formed in a flat one-body band. Furthermore we perform DMRG simulations and exact diagonalization, and present strong evidence for the energetic stability of the multimer states with \( N = \{2, 3, \cdots, 10\} \), conceivably without an upper bound on \( N \) and with a quasi-flat \((N + 1)\)-body dispersion. Given the recent surge of experimental and theoretical interest in flat-band systems \([30–42]\), we hope that our peculiar findings will trigger further interest in the few-body aspects of Kagome and Lieb-like toy models that exhibit a flat band in their one-body-spectrum \([43]\).

Multiband Hubbard Model: The standard Hubbard Hamiltonian \([38, 44]\) \( \mathcal{H} = \sum_{\sigma} \mathcal{H}_{\sigma} + \mathcal{H}_{t1} \) is made of two terms:

\[
\mathcal{H}_{\sigma} = - \sum_{Si:Si'} t_{Si:Si'}^\sigma c_{Si}\sigma^\dagger c_{Si'}\sigma, \tag{1}
\]

\[
\mathcal{H}_{t1} = -U \sum_{Si} c_{Si}\uparrow^\dagger c_{Si}\uparrow^\dagger c_{Si}\downarrow c_{Si}\downarrow. \tag{2}
\]

Here the first term accounts for the kinetic energy of the spin-\(\sigma\) fermions where the hopping parameter \( t_{Si:Si'}^\sigma \) describes their tunneling amplitude from the sublattice (or basis or orbital) site \( S' \) in the unit cell \( i' \) to the sublattice site \( S \) in the unit cell \( i \). On the other hand the second term accounts for the potential energy of the system, where \( U \geq 0 \) is the strength of the attractive in-
teration between $\uparrow$ and $\downarrow$ fermions when they are on the same site. Next we use a canonical transformation, i.e., $c^\dagger_{S\sigma} = \frac{1}{\sqrt{N_c}} \sum_k e^{-ik\cdot r_{Si}} c^\dagger_{Sk\sigma}$, and express the Hubbard Hamiltonian in the reciprocal lattice, where $N_c$ is the number of unit cells in the system, $\mathbf{k}$ is the crystal momentum in the first Brillouin zone (BZ), and $r_{Si}$ is the position of the sublattice site $S$ in unit cell $i$. Note that the total number of lattice sites is $N_s = N_b N_c$ when the number of sublattice sites in a unit cell is $N_b$. In addition noting that $c^\dagger_{Sk\sigma} = \sum_S n_{Sk\sigma} c^\dagger_{Sk\sigma} c_{nK\sigma}$, where $n$ is the band index for the Bloch bands (there are $N_b$ of them) and $n_{Sk\sigma}$ is the projection of the Bloch state onto the sublattice $S$, we eventually find [28]

$$\mathcal{H}_o = \sum_{nK} \varepsilon_{nK} c^\dagger_{nK\sigma} c_{nK\sigma},$$  

(3)

$$\mathcal{H}_{\uparrow\downarrow} = \frac{1}{N_c} \sum_{n'm'} \sum_{kk} \sum_{m'n'} V_{n'm'k}(q) b^\dagger_{nm}(k,q)b_{n'm'}(k',q).$$  

(4)

Here $\varepsilon_{nK\sigma}$ is the one-body dispersion of the fermions in band $n$, $V_{n'm'k}(q) = -U \sum_S n_{Sk+k+\frac{3}{2}\uparrow} m_{Sk+k+\frac{3}{2}\downarrow} m_{Sk+k+\frac{3}{2}\downarrow} m_{Sk+k+\frac{3}{2}\uparrow}$ characterizes the onsite interactions in momentum space, and $b^\dagger_{nm}(k,q) = c^\dagger_{n,S,k+\frac{3}{2}\uparrow} c_{m,-k+\frac{3}{2}\downarrow}$ creates a pair of fermions in the Bloch bands.

$(N+1)$-Body Problem: In this paper we are interested in the role of multiple Bloch bands on the energetic stability of the multimeter states. For this purpose we consider few-body bound states that are made of $N$ spin-$\uparrow$ fermions and a single spin-$\downarrow$ fermion. Motivated by the success of variational approach on the two-body and three-body problems [27–29], here we attack the $(N+1)$-body problem with the following ansatz

$$\mathcal{H}|\Psi_q\rangle = E_{N+1}^q|\Psi_q\rangle,$$  

(5)

$$|\Psi_q\rangle = \sum_{n_1 \cdots n_{N+1}} \alpha_{n_1 \cdots n_{N+1} m}(q) \left( \prod_{i=1}^{N+1} c^\dagger_{n_i k_i \uparrow} \right) |0\rangle.$$  

(6)

Here the ansatz $|\Psi_q\rangle$ explicitly conserves the center-of-mass momentum $q$ of the particles, $E_{N+1}^q$ is the energy of the $(N+1)$-body state, $\alpha_{n_1 \cdots n_{N+1} m}(q)$ is the variational complex bound parameter, and $Q = q - \sum_{i=1}^{N} k_i$ is defined for convenience. Since $|\Psi_q\rangle$ has the most general form, it will provide us the exact solution. The normalization condition can be written as $\langle \Psi_q | \Psi_q \rangle = N! \sum_{n_1 \cdots n_{N+1}} |\alpha_{n_1 \cdots n_{N+1} m}(q)|^2$, where we enforce the Pauli principle, and make extensive use of $\delta_{n_1 \cdots n_{N+1} \uparrow \uparrow\downarrow \downarrow}$, i.e., the ansatz picks up a minus sign under the exchange of a pair of its spin-$\uparrow$ fermions. After a lengthy but a straightforward calculation, we find

$$\langle \mathcal{H}_\uparrow \rangle = N! \sum_{n_1 \cdots n_{N+1} m} |\alpha_{n_1 \cdots n_{N+1} m}(q)|^2 \left( \sum_{i=1}^{N} \varepsilon_{n_i k_i \uparrow} \right),$$  

(7)

$$\langle \mathcal{H}_\downarrow \rangle = N! \sum_{n_1 \cdots n_{N+1} m} |\alpha_{n_1 \cdots n_{N+1} m}(q)|^2 \varepsilon_{m q},$$  

(8)

$$\langle \mathcal{H}_{\uparrow\downarrow} \rangle = \frac{-N!U}{N_c} \sum_{n_1 \cdots n_{N+1} m} \alpha_{n_1 \cdots n_{N+1} m}(q) \sum_{Sk \in k_{\uparrow\downarrow}} \alpha_{n_S k_{\uparrow\downarrow}} \delta_{k_{\uparrow\downarrow}},$$  

(9)

for the expectation value of the multiband Hubbard Hamiltonian. Here $^*$ is for the complex conjugation and $\delta_{ij}$ is the Kronecker delta.

The variational parameters are determined through the functional minimization of $\langle \Psi_q | \mathcal{H} - E_{N+1}^q | \Psi_q \rangle$, but this procedure leads to a complicated expression. In order to simplify the resultant equations, we define a new parameter set

$$\alpha_{n_1 \cdots n_{N+1} m}(q) = \sum_{n_1 \cdots n_{N+1}} \alpha_{n_1 \cdots n_{N+1} m}(q) n_1 \delta_{k_{\uparrow\downarrow}} m_S Q_{\uparrow\downarrow},$$  

(10)

and make use of Pauli exchange statistics $\delta_{k_{\uparrow\downarrow}} k_{\uparrow\downarrow} \delta_{k_{\uparrow\downarrow}} \delta_{k_{\uparrow\downarrow}}$.

Finally, we finnally obtain a set of coupled integral equations with the following structure

$$\alpha_{n_1 \cdots n_{N+1} m}(q) = \sum_{n_1 \cdots n_{N+1}} \alpha_{n_1 \cdots n_{N+1} m}(q) n_1 \delta_{k_{\uparrow\downarrow}} m_S Q_{\uparrow\downarrow},$$  

(11)

This exact expression is one of our central results in this work: the $(N+1)$-body problem in a multiband Hubbard model is reduced to the solutions of $N_b^N$ coupled integral equations with $N - 1$ momentum variables for a given
set of parameters, i.e., \( q, U \) and hoppings. Its continuum version is recovered by setting the Bloch factors to unity and dropping the band as well as sublattice indices, i.e., it requires the solution of a single integral equation for \( \gamma_{k_2:k_3}(q) \), see Eq. (3) in Ref. [19], and Ref. [45] for details. Once \( E^b_{N+1} \) is obtained, the binding energy of the \((N+1)\)-body bound state can be determined by

\[
E_{N+1}^b(q) = -E^b_{N+1} + \min\{E^\ell_{(N+1)-1} + \varepsilon_n q - q' \uparrow\}. \tag{12}
\]

This is because while an \((N+1)\)-body bound state may in general become energetically unstable against dissociation into an \([(N - \ell) + 1]\)-body bound state and \( \ell \) free spin-\( \uparrow \) fermions, the \( \ell = 1 \) process is closest in energy to \( E^\ell_{N+1} \) when the \([(N - 1) + 1]\)-body bound state is energetically-stable, i.e., \( E^\ell_{N}(q) > 0 \), to begin with [46]. Indeed this turns out to be the case for all of the multimers in the flat-band of sawtooth lattice discussed below.

Let’s first show that Eq. (11) reproduces the available literature in the \( N = 1 \) and \( N = 2 \) cases. For \( N = 1 \), since the summation term of the second line is irrelevant, Eq. (11) is equivalent to

\[
\gamma^S(q) = \sum_{n_{1,mS}k_1} \frac{m^S_{Q}\pi m^S_{Q}n_{1}^{S}k_1^{\dagger}n_{1}^{S}k_1^{+}}{\varepsilon_{n_{1}k_1^{\dagger}} + \varepsilon_{n_{1}mQ} - E^q} \gamma^S(q), \tag{13}
\]

where \( Q = q - k_1 \). This self-consistency relation can be recast as an eigenvalue problem of an \( N_b \times N_b \) matrix, giving rise to \( N_b \) branches for the two-body dispersion \( E^S_{2} \) for each given \( q \). See Ref. [26] for an alternative derivation with a different approach. Equation (13) is recently used to reveal a deeper connection between the effective-mass tensor of the lowest-lying dimer states and the quanum-metric tensor of the underlying Bloch states [28, 29, 47].

For \( N = 2 \) Eq. (11) reduces to

\[
\gamma^S_{n_{2}S}(q) = \sum_{n_{1,mS}k_1} \frac{m^S_{Q}\pi m^S_{Q}n_{1}^{S}k_1^{\dagger}n_{1}^{S}k_1^{+}}{\varepsilon_{n_{1}k_1^{\dagger}} + \varepsilon_{n_{1}mQ} - E^q} \times [n_{2}^{S}\gamma^S_{n_{2}S}(q) - n_{2}^{S}k_1^{\dagger}\gamma_{n_{1}S}(q)], \tag{14}
\]

where \( Q = q - k_1 - k_2 \). This is a set of \( N_b^2 \) coupled integral equations with one momentum variable, and it can be recast as an eigenvalue problem of an \( N_b^2 \times N_b^2 \) matrix for each given \( q \). Equation (14) has recently been derived by one of us [27], and its numerical solutions for \( E^S_{3} \) are in excellent agreement with the DMRG simulations in a sawtooth lattice [26]. In particular, in sharp contrast with the exact results on the single-band linear-chain model which dismiss trimers [6, 20, 21, 25], it is found that the presence of an additional band allows the formation of energetically-stable trimer states in the sawtooth lattice. In addition it is found that the trimers have a quasi-flat dispersion when formed in a flat band, which is unlike the highly-dispersive spectrum of its dimers. These surprising results are one of the main motivations for the current work, i.e., we want to study the stability of larger few-body clusters in the presence of multiple bands.

Let’s next consider the four-body problem and study the fate of tetramer bound states. For \( N = 3 \) Eq. (11) reduces to

\[
\gamma^S_{n_{2}n_{3}S}(q) = \sum_{n_{1,mS}k_1} \frac{m^S_{Q}\pi m^S_{Q}n_{1}^{S}k_1^{\dagger}n_{1}^{S}k_1^{+}}{\varepsilon_{n_{1}k_1^{\dagger}} + \varepsilon_{n_{1}mQ} - E^q} \times [n_{2}^{S}\gamma^S_{n_{2}n_{3}S}(q) - n_{2}^{S}k_1^{\dagger}\gamma_{n_{1}S}(q) - n_{3}^{S}\gamma^S_{n_{2}n_{3}S}(q)], \tag{15}
\]

where \( Q = q - k_1 - k_2 - k_3 \). This is a set of \( N_b^3 \) coupled integral equations with two momentum variables, and it can be recast as an eigenvalue problem of an \( N_b^3 \times N_b^3 \) matrix for each given \( q \). Our numerical recipe is provided in the supplementary material [48]. In this work we apply Eq. (15) to the sawtooth model due in part to its flat-one-body and one-dimensional simplicity, and most importantly to our benchmarking capacity with the DMRG simulations and exact diagonalization.

**Sawtooth Lattice:** Due to the presence of its \( N_b = 2 \) sublattice sites in a unit cell (say \( S = \{A, B\} \) sublattices), the sawtooth lattice features a one-body bound state with two Bloch bands in the first BZ (say \( s = \{+,-\} \) bands). See the inset of Fig. 1(a) for its sketch. Here we allow hopping between nearest-neighbor sites only, and set \( t_{Aj:Bi}^s = -t \) with \( j = \pm 1 \) and \( t \geq 0 \), \( t_{Bi:Bj}^- = 0 \) and \( t_{Bi:Bj}^+ = t_{Bj:Bi}^- = -t' \) with \( j = \pm 1 \) and \( t' \geq 0 \). Thus the one-body Hamiltonian can be written as

\[
\mathcal{H}_s = \sum_k \psi_{k\sigma}^\dagger \left( d_k^0 \sigma_0 + d_k \cdot \sigma \right) \psi_{k\sigma}, \tag{16}
\]

where \( \psi_{k\sigma} = (c_{Ak\sigma} c_{Bk\sigma})^T \) is a spinor, \(-\pi/a < k \leq \pi/a \) is the first BZ, \( d_k^0 = t \cos(ka), \sigma_0 = 1 \times 2 \) identity matrix, \( d_k = (d_k^+ d_k^-) \) is a field vector with elements \( d_k^+ = t' + t \cos(ka) \), \( d_k^- = t' \sin(ka) \) and \( d_k^z = t \cos(ka) \), and \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) is a vector of Pauli spin matrices. The one-body dispersions can be written as \( \varepsilon_{sk\sigma} = d_k^z + s d_k \) where \( s = \pm \) for the upper and lower bands, respectively, and \( d_k \) is the magnitude of \( d_k \). The sublattice projections of the corresponding eigenvectors are \( s_{Ak\sigma} = (d_k^x + id_k^y)/\sqrt{2d_k(d_k - sd_k^z)} \) and \( s_{Bk\sigma} = (d_k^z - sd_k)/\sqrt{2d_k(d_k - sd_k^z)} \). One of the most treasured features of this toy model is the presence of a flat (lower) band \( \varepsilon_{-,k} = -2t \) in its dispersion when \( t'/t = \sqrt{2} \) [26, 27, 49–51].

Our variational results for \( E^S_2 \) and \( E^S_3 \) are presented, respectively, in Figs. 1(a) and 1(b), where we use a \( k \)-space mesh with \( N_c = 30 \) points and checked that using \( N_c = 50 \) points makes minor corrections. Indeed the ground-state energy of the tetramers is typically within 1\% relative accuracy with the DMRG simulations (see below). One of our main findings is that the four-body dispersion \( E^S_4 \) is quasi-flat (with a negligible bandwidth).
when the tetramers are formed in a flat one-body band, i.e., when $t'/t = \sqrt{2}$. For instance $U = 5t'$ is shown in Fig. 1(a), and we found similar results for lower and higher $U/t'$ values as well (not shown). It is conceivable that the tetramers have a respectable dispersion in the weak-coupling limit when $U/t' \lesssim 1$, but our numerical calculations are not expected to be as reliable there. This is because one needs to use a much higher $N_c$ as the size (in real space) of the bound states gets much larger in the $U/t' \to 0$ limit. We also calculated the binding energy $E_{4c}^1(q)$ of the tetramers and verified their energetic stability: e.g., we found that $E_{4c}^1(q)$ becomes positive as soon as $U \neq 0$ when the tetramers are formed in a flat one-body band. However this is not the case when $t'/t \neq \sqrt{2}$, i.e., $E_{4c}^1(q)$ becomes positive beyond a critical threshold on $U$ in such a way that larger deviations from the flat-band case leads to a higher threshold.

**Pentamers and Beyond:** For $N \geq 4$ it is possible to solve Eq. (11) again by recasting it as an eigenvalue problem, but such a numerically-expensive task is beyond our capacity. Instead here we present our numerical results from the DMRG simulations [52–54] and exact diagonalization [55]. For this purpose we define the ground-state binding energy of the $(N+1)$-body bound state as

$$E_{N+1}^{be}(gs) = -E_0(N,1) + E_0(N-1,1) + E_0(1,0),$$  

(17)

where $E_0(N_1, N_2)$ is the ground-state energy of the $(N_1+N_2)$-body problem. Given the definition in Eq. (12), Eq. (17) is strictly valid under the assumption that the center-of-mass momentum of the ground-state of the $(N+1)$-body problem is equal to the total momentum of the ground-states of the $[(N-1)+1]$-body and one-body problems. Unlike the $t'/t < \sqrt{2}$ case where the ground-state of the one-body problem is at the edge of the BZ, our variational results suggest that this requirement is usually fulfilled when $t'/t \geq \sqrt{2}$.

In Fig. 2(a) we set $t'/t = \{\sqrt{2}, \sqrt{3}\}$, and present the DMRG results for $E_{N+1}^{be}(gs)$ as a function of $U/t'$. Here we use a long lattice with $N_s = 100$ sites and with open boundary conditions. We only show $N = \{1, 2, \cdots , 7\}$ since the accuracy of our DMRG simulations does not allow us to resolve $E_{N+1}^{be}(gs)$ for the entire $U/t'$ range when $N \geq 8$. To overcome this limitation, we also perform the exact diagonalization of a fairly large lattice with $N_s = 22$ sites, and they are presented in Fig. 2(b) for $N = \{1, 2, \cdots , 10\}$. First of all the variational, DMRG and exact diagonalization approaches are in very good agreement with each other when they have an overlap at low $N_c$ values. For $N \geq 2$ they suggest the presence of larger and larger few-body clusters with lower and lower binding energies, conceivably without an upper bound on $N$ [56]. In addition all of these clusters are energetically stable when formed in a flat one-body band, i.e., $E_{N+1}^{be}(gs) > 0$ as soon as $U \neq 0$. Unlike $E_2^{be}(gs)$ of the dimer that grows linearly with $U$ in the strong-coupling limit when $U/t' \gg 1$, we note that $E_{N+1}^{be}(gs)$ always saturates for $N \geq 2$, i.e., it fits quite well with $C_{N}' t' - C_{N}'' t'^2 / U$ where $C_N'$ and $C_N''$ both decay rapidly with $N$. In addition we also checked the energies of the first few excited states in our exact diagonalization studies. For instance, as shown in the supplementary materials [48], the energy gaps between the first few excited states and the ground state vanish exactly when $t'/t = \sqrt{2}$. Thus it is also conceivable that some of the lowest-lying $(N+1)$-body bound states have quasi-flat dispersions in the BZ when formed in a flat one-body band.

**Conclusion:** In summary here we used variational, DMRG and exact diagonalization approaches, and studied the bound states of $N$ identical spin-$\uparrow$ fermions and a single spin-$\downarrow$ fermion in a generic multiband Hubbard Hamiltonian with onsite attractive interactions. In the case of a sawtooth lattice with a flat one-body band, we showed strong evidence for the existence of energetically-stable few-body clusters with $N = \{2, 3, \cdots , 10\}$, conceivably without an upper bound on $N$ and with a quasi-flat $(N+1)$-body dispersion in the first BZ. These pecu-
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It is such that the binding energy $E_{\text{be}}^{\uparrow\downarrow}(q)$ of the dimer is always defined from an unbound pair of a free spin-$\uparrow$ fermion plus a free spin-$\downarrow$ fermion; the binding energy $E_{\text{be}}^{\uparrow\downarrow}(q)$ of the tetramer is defined from the trimer threshold plus a free spin-$\uparrow$ fermion when $E_{\text{be}}^{\uparrow\downarrow}(q) > 0$, etc.

P. Törmä, L. Liang, and S. Peotta, Quantum metric and effective mass of a two-body bound state in a flat band, Phys. Rev. B 98, 220511 (2018).

See Supplementary Material (A) for the numerical implementation of the four-body problem from the variational approach, and (B,C) for additional results from the DMRG simulations and exact diagonalization.

H. Tasaki, From nagaoka’s ferromagnetism to flat-band ferromagnetism and beyond: An introduction to ferromagnetism in the Hubbard model, Prog. Theor. Phys. 99, 489 (1998).

V. A. J. Pyykknen, S. Peotta, P. Fabritius, J. Mohan, T. Esslinger, and P. Trm, Flat-band transport and Josephson effect through a finite-size sawtooth lattice, Phys. Rev. B 103, 144519 (2021).

S. M. Chan, B. Grmaud, and G. G. Batrouni, Pairing and superconductivity in quasi-one-dimensional flat-band systems: Creutz and sawtooth lattices, Phys. Rev. B 105, 024502 (2022).

S. R. White, Density matrix formulation for quantum renormalization groups, Phys. Rev. Lett. 69, 2863 (1992).

U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, Ann. Phys. 326, 96 (2011).

M. Fishman, S. R. White, and E. M. Stoudenmire, The ITensor software library for tensor network calculations (2020), arXiv:2007.14822.

P. Weinberg and M. Bukov, QuSpin: a Python Package for Dynamics and Exact Diagonisation of Quantum Many Body Systems. Part II: bosons, fermions and higher spins, SciPost Phys. 7, 20 (2019).

A plausible mechanism for the appearence of energetically-stable $(N + 1)$-body bound states in a flat band is as follows: when the spin-$\uparrow$ fermions are localized on the nearest-neighbor sites (due to their diverging effective band mass), the delocalization of the spin-$\downarrow$ fermion on these sites might be favored by the onsite attraction in between. This can be achieved through interband transitions with the upper band, reducing the overall energy of the system. We note that a similar interband mechanism (that is mediated by $U \neq 0$) is fully responsible for the finite effective-mass of the low-energy dimers when they are formed in a flat one-body band [26, 28, 29, 47]. In this scenario the spin-$\downarrow$ fermion can hop between spin-$\uparrow$ fermions only through dissociation of the virtual dimers, and this process leads to an effective hopping that scales as $\sim C_N t^2 / E_{\text{be}}^{\uparrow\downarrow}(gs)$ where $C_N$ depends on $N$. This further suggests that $E_{\text{be}}^{N,1}(gs) \sim C_N t^2 - C_N t^2 / U$ in the strong-coupling limit when $U/t > 1$ because $E_{\text{be}}^{\uparrow\downarrow}(gs) \rightarrow U$ in this limit. Indeed this turns out to be the case in our exact diagonalization results that are shown in the supplementary materials.
SUPPLEMENTARY MATERIAL

A: Numerical implementation of the (3 + 1)-body problem

Equation (15) is a set of $N_b^3$ coupled integral equations with two momentum variables, and here we show how to recast it as an eigenvalue problem of an $N_b^3 N_c^2 \times N_b^3 N_c^2$ matrix for each given $q$. First we rewrite Eq. (15) as

$$\gamma_{nmS}(q) = \sum_{S'} f_{nmS;nS'}^{qkk'} \gamma_{nmS}(q) + \sum_{n'm'S'} g_{nmS;n'm'S'}^{qkk'} \gamma_{nmS}(q) + \sum_{n'm'S'} h_{nmS;n'm'S'}^{qkk'} \gamma_{nmS}(q),$$

whose coefficients $f_{nmS;nS'}^{qkk'}, g_{nmS;n'm'S'}^{qkk'}$, and $h_{nmS;n'm'S'}^{qkk'}$, are stored as

$$f_{nmS;nS'}^{qkk'} = \frac{U}{N_c} \sum_{n,m,p} \frac{m'^*_{S} K_{s} m'_{S_k} n'_{S_p} p_{S'^*} }{\varepsilon_{nk} + \varepsilon_{mk} + \varepsilon_{n'p} + \varepsilon_{m'k} - E_4},$$

$$g_{nmS;n'm'S'}^{qkk'} = -\frac{U}{N_c} \frac{m'^*_{S} K_{s} m'_{S_k} n'_{S_p} p_{S'^*} }{\varepsilon_{nk} + \varepsilon_{mk} + \varepsilon_{n'p} + \varepsilon_{m'k} - E_4},$$

$$h_{nmS;n'm'S'}^{qkk'} = -\frac{U}{N_c} \frac{m'^*_{S} K_{s} m'_{S_k} n'_{S_p} p_{S'^*} }{\varepsilon_{nk} + \varepsilon_{mk} + \varepsilon_{n'p} + \varepsilon_{m'k} - E_4}.$$

Here we defined $K = q - k - k' - p$ for convenience. Then we define an $N_b^3$-component vector, e.g.,

$$\gamma_{kk'(q)} = \begin{bmatrix} \gamma_{11A}^{kk'}(q) & \gamma_{11B}^{kk'}(q) & \gamma_{12A}^{kk'}(q) & \gamma_{12B}^{kk'}(q) & \gamma_{21A}^{kk'}(q) & \gamma_{21B}^{kk'}(q) & \gamma_{22A}^{kk'}(q) & \gamma_{22B}^{kk'}(q) \end{bmatrix}^T$$

in the case of a lattice with two sublattice sites, i.e., $N_b = 2$. Here $n = \{1, 2\}$ is the band index, $S = \{A, B\}$ is the sublattice index, and $T$ is the transpose. Equation (18) can be written as

$$\gamma_{kk'}(q) = f_{q}^{kk'} \gamma_{kk'}(q) + \sum_{p} G_{q}^{kk'p} \gamma_{pk'}(q) + \sum_{p} H_{q}^{kk'p} \gamma_{kp}(q)$$
Finally we use the underlying k-space mesh in the first BZ, i.e., \( k = \{ k_1, k_2, \cdots, k_{N_k} \} \), and define an \( N_k^3 N_q^2 \)-component vector with the following elements

\[
\Gamma_q = [ \gamma_{k_1 k_2} (q) \gamma_{k_1 k_2} (q) \cdots \gamma_{k_1 k_{N_k}} (q) \gamma_{k_2 k_1} (q) \gamma_{k_2 k_2} (q) \cdots \gamma_{k_2 k_{N_k}} (q) \gamma_{k_3 k_1} (q) \cdots \gamma_{k_{N_k} k_{N_k}} (q) ]^T.
\]

(27)

Equation (23) can be written as

\[
(\mathbf{F}_q + \mathbf{G}_q + \mathbf{H}_q) \Gamma_q = \Gamma_q,
\]

(28)
where $F_q$, $G_q$, and $H_q$ are $N_q^3 N_c^2 \times N_q^3 N_c^2$ matrices with the following elements:

$$
F_q = \begin{pmatrix}
F_{q}^{k_1 k_1} & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots \\
0 & F_{q}^{k_1 k_1} & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
0 & 0 & \cdots & F_{q}^{k_1 k_{N_c}} & 0 & 0 & \cdots & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & F_{q}^{k_2 k_1} & 0 & \cdots & 0 & 0 & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & F_{q}^{k_2 k_{N_c}} & 0 & \cdots \\
0 & 0 & \cdots & 0 & 0 & \cdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
\end{pmatrix}
$$

(29)

$$
G_q = \begin{pmatrix}
G_{q}^{k_1 k_1 k_1} & 0 & \cdots & 0 & G_{q}^{k_1 k_1 k_2} & 0 & \cdots & 0 & G_{q}^{k_1 k_1 k_3} & 0 & \cdots & 0 \\
0 & G_{q}^{k_1 k_1 k_1} & \cdots & 0 & 0 & G_{q}^{k_1 k_1 k_2} & \cdots & 0 & 0 & G_{q}^{k_1 k_1 k_3} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & G_{q}^{k_1 k_{N_c} k_1} & 0 & 0 & \cdots & G_{q}^{k_1 k_{N_c} k_2} & 0 & 0 & \cdots & G_{q}^{k_1 k_{N_c} k_3} \\
G_{q}^{k_2 k_1 k_1} & 0 & \cdots & 0 & G_{q}^{k_2 k_1 k_2} & 0 & \cdots & 0 & G_{q}^{k_2 k_1 k_3} & 0 & \cdots & 0 \\
0 & G_{q}^{k_2 k_1 k_1} & \cdots & 0 & 0 & G_{q}^{k_2 k_1 k_2} & \cdots & 0 & 0 & G_{q}^{k_2 k_1 k_3} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & G_{q}^{k_2 k_{N_c} k_1} & 0 & 0 & \cdots & G_{q}^{k_2 k_{N_c} k_2} & 0 & 0 & \cdots & G_{q}^{k_2 k_{N_c} k_3} \\
G_{q}^{k_3 k_1 k_1} & 0 & \cdots & 0 & G_{q}^{k_3 k_1 k_2} & 0 & \cdots & 0 & G_{q}^{k_3 k_1 k_3} & 0 & \cdots & 0 \\
0 & G_{q}^{k_3 k_1 k_1} & \cdots & 0 & 0 & G_{q}^{k_3 k_1 k_2} & \cdots & 0 & 0 & G_{q}^{k_3 k_1 k_3} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & G_{q}^{k_3 k_{N_c} k_1} & 0 & 0 & \cdots & G_{q}^{k_3 k_{N_c} k_2} & 0 & 0 & \cdots & G_{q}^{k_3 k_{N_c} k_3} \\
\end{pmatrix}
$$

(30)

$$
H_q = \begin{pmatrix}
H_{q}^{k_1 k_1 k_1} & H_{q}^{k_1 k_1 k_2} & \cdots & H_{q}^{k_1 k_1 k_{N_c}} & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots \\
H_{q}^{k_1 k_1 k_2} & H_{q}^{k_1 k_1 k_2} & \cdots & H_{q}^{k_1 k_1 k_{N_c}} & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \\
H_{q}^{k_1 k_{N_c} k_1} & H_{q}^{k_1 k_{N_c} k_2} & \cdots & H_{q}^{k_1 k_{N_c} k_{N_c}} & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & H_{q}^{k_2 k_1 k_1} & H_{q}^{k_2 k_2 k_2} & \cdots & H_{q}^{k_2 k_2 k_{N_c}} & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & H_{q}^{k_2 k_1 k_1} & H_{q}^{k_2 k_2 k_2} & \cdots & H_{q}^{k_2 k_2 k_{N_c}} & 0 & 0 & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \\
0 & 0 & \cdots & 0 & H_{q}^{k_2 k_{N_c} k_1} & H_{q}^{k_2 k_{N_c} k_2} & \cdots & H_{q}^{k_2 k_{N_c} k_{N_c}} & 0 & 0 & \cdots \\
0 & 0 & \cdots & 0 & H_{q}^{k_3 k_1 k_1} & H_{q}^{k_3 k_1 k_2} & \cdots & H_{q}^{k_3 k_1 k_{N_c}} & 0 & 0 & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \\
\end{pmatrix}
$$

(31)

Thus the four-body problem reduces to the solutions of an eigenvalue problem defined by Eq. (28). It can be solved numerically by iterating $E_{d}^q$ until one of the eigenvalues of $F^q + G^q + H^q$ becomes exactly 1. Typically there are many $E_{d}^q$ solutions for a given set of lattice parameters. In this work we are interested in those tetramer states with lowest energy for a given $q$. 
B: Energy gaps from the exact diagonalization

![Graph showing energy gaps for different N and t’/t values for U/t’ = 5.0 and 15.0](image)

FIG. 3. Energy gaps from the exact diagonalization of a lattice with Ns = 22 sites. Upper and lower panels correspond, respectively, to U/t’ = 5 and U/t’ = 15. For N = {2, 3, 4, ···, 6} the energy gaps between the first three excited states and the ground state vanish exactly at t’/t = √2. On the other hand, when the cluster size (i.e., N + 1) becomes comparable to the number of states in a flat band (i.e., Nc = Ns/2), one expects large energy gaps to appear due to finite-size effects even at t’/t = √2. Here they clearly appear for N ≥ 7. In the light of these results and assuming much larger lattices, it is conceivable that some of these (N + 1)-body bound states have quasi-flat dispersions when formed in a flat one-body band. It is important to remark here that the (N + 1)-body bound states may not be energetically stable for all N when t’/t ≠ √2, e.g., see Fig.2(a) of the main text for the t’/t = √3 case where N ≥ 5 are not stable.

C: Strong-coupling limit when U/t’ → ∞
FIG. 4. Binding energies $E_{N+1}^{be}(gs)$ from exact diagonalization with $N_s = 22$ sites for $t'/t = \sqrt{2}$. The strong-coupling limit $t'/U \ll 1$ seems to fit quite well with $E_{N+1}^{be}(gs)/t' = \varepsilon_0 + \varepsilon_1(t'/U) + \varepsilon_2(t'/U)^2$ for all $N \geq 2$, where the saturation point $\varepsilon_0$ at $t'/U \to 0$ decreases rapidly with $N$. It is also shown that the fit $\varepsilon_0 \sim 4.43e^{-1.14N+0.04N^2}$ matches reasonably well with the available data for $N = \{2, 3, \cdots, 10\}$. 