Signatures of the BCS-BEC crossover in the yrast spectra of Fermi quantum rings

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We study properties of the lowest energy states at non-zero total momentum (yrast states) of the Hubbard model for spin-$\frac{1}{2}$ fermions in the quantum ring configuration with attractive on-site interaction at low density. In the one-dimensional (1D) case we solve the Hubbard model using the Bethe ansatz, while for the crossover into the 2D regime we use the Full-Configuration-Interaction Quantum Monte-Carlo method (FCIQMC) to obtain the yrast states for the spin-balanced Fermi system. We show how the yrast excitation spectrum changes from the 1D to the 2D regime and how pairing affects the yrast spectra. We also find signatures of fragmented condensation for certain yrast states usually associated with dark solitons.

I. INTRODUCTION

The crossover from a fermionic superfluid of weakly-bound Cooper pairs (BCS regime) to a Bose-Einstein condensate (BEC) of strongly-bound dimers is a paradigmatic quantum many-body problem [14]. Our understanding of this problem is still limited, as strong quantum correlations and the absence of a small parameter pose severe challenges for theoretical and computational approaches. While bulk systems have been studied extensively in recent years using theory [8-10] and experiments with quantum gases [11-15], the advent of quantum gas microscopes [16-19] and micro traps [20-23] has opened up the opportunity to experiment with systems that are small enough to perform exact numerical calculations on.

Of particular interest are ring configurations, where translational invariance along one spatial dimension makes (angular) momentum a good quantum number. This allows for the study of yrast states, which are defined as the lowest energy state at given value of the total momentum. Yrast states in a bosonic superfluid are intimately connected to localized nonlinear waves known as dark solitons [32]. It was shown that measuring the position of all bosons in an yrast state reveals a dark-soliton-like particle depletion [39], and that wave-packet-like superpositions of yrast states emulate the behavior of classical dark solitons [31]. While the yrast states are fragmented quantum condensates, breaking the translational symmetry restores single condensation and classical soliton features [28]. Dark solitons in Fermi superfluids have been identified in experiments [34-35], but many predictions from mean-field theory have not yet been tested [29-32]. Moreover, there is an intriguing connection [33, 44] between dark solitons and the predicted Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase of imbalanced superfluids [45, 46]. Dispersion relations of yrast states were analyzed in the context of dark soliton physics in the Yang-Gaudin model, a one-dimensional (1D) Bethe-ansatz solvable model of a fermionic superfluid in Ref. [47]. An overview of computational studies of quantum rings can be found in the recent review literature [48, 50].

Beyond the purely one-dimensional models of quantum rings, a second spatial dimension can be added by considering stripe- or ladder-type lattice configurations that are small enough to perform exact numerical calculations on, but they fix the chemical potential instead of particle number and the number of lattice sites. Quantum Monte Carlo (QMC) simulations are still possible, although the fermion sign problem [51, 52] provides a challenge for the simulation of fermionic many-body problems.

QMC methods relevant in the field of ultracold quantum gases each have their own strengths and weaknesses. Diffusion Monte Carlo has no basis set dependence but either converges to a bosonic ground state or requires node-fixing, which introduces an approximation [53]. Auxiliary-field QMC is sign-problem free for the attractive balanced Hubbard model [54], but the Hubbard-Stratonovich transformation involved in this method breaks symmetries of the Hamiltonian and thus does not allow for the study of yrast states. Recent work has suggested a solution [55], but it has yet to be seen whether the method can be implemented efficiently. Determinant Monte Carlo and related methods can handle finite temperature and extrapolate to zero temperature, but they fix the chemical potential instead of particle number [56, 59]. All these existing methods have in common that they can study overall ground-state properties while it is not possible to study yrast states, because the
total momentum cannot be easily constrained.

For this work we use Full-Configuration-Interaction Quantum Monte Carlo (FCIQMC), a method originally developed for strongly correlated electrons in the context of quantum chemistry \[60, 61\]. FCIQMC has been applied with great success to a large number of problems in this field \[62, 63\], and recently to ultracold atoms \[64, 65\]. This method can find the ground state energy and many-body wave function in a Fermi system by expanding the wave function into a set of Slater determinants. A stochastic version of exact diagonalization of the Hamiltonian in this basis is achieved by simulating the dynamics of a walker population in Slater determinant space. FCIQMC mitigates the sign problem by walker annihilation to a certain degree but does not eliminate it \[66\]. By performing a stochastic projection to the ground state of a Hamiltonian in a given Fock basis directly, i.e. without resorting to a Hubbard-Stratonovich transformation, it is easy to respect symmetries of the Hamiltonian. In particular, it is possible to obtain energies and observables from yrast states by ground state projection in a plane-wave basis because the FCIQMC algorithm conserves total momentum if the Hamiltonian does. With the FCI method taking into account all correlations in the system, we probe the BCS-BEC crossover in the excitation energy and many-body wave function in a Fermi system at the so-called “umklapp” points where sufficient quasi-momentum is added to boost either all or half of the constituent fermions by one unit in order to form a ring current. We find signatures of the transition from non-interacting Fermi gas to a paired superfluid and of the BCS to BEC crossover in the excitation energy and in the pair correlation functions for the first half and full umklapp points. Last, we focus on the yrast states around the maxima of the dispersion, which are related to dark solitons. We calculate the inertial mass of possible solitons for different system sizes and interaction strengths. We find an increase of the inertial mass by a factor of 2 when the transverse dimension is large enough for the system to be considered truly 2D, which is indicative of a transition from dark soliton to a solitonic vortex \[67, 68\]. From mean-field and basic hydrodynamic theory, in the 1D to 2D crossover dark solitons are replaced as stable yrast excitations by solitonic vortices \[66, 69\], or vortex pairs \[41, 70\], which have larger inertial mass \[31, 71, 72\]. By looking at the pair densities of these yrast states, we find that fragmented condensation into more than one momentum state takes place, as expected for superfluid yrast states \[28\].

This paper is organized as follows: After introducing the model in Sec. II and the FCIQMC approach in Sec. III we discuss yrast spectra of a 1D Hubbard chain obtained by the Bethe ansatz in Sec. IV. The energies and spin correlation functions for the umklapp points in the 1D to 2D crossover are discussed in Sec. V before analysing the physics of the maxima of the yrast dispersion by computing their effective mass and momentum-space pair densities in Sec. VI and drawing conclusions in Sec. VII.

II. SYSTEM

To study yrast states in an ultracold fermionic superfluid, we use the Hubbard model in the regime of low densities. In this regime, the Hubbard model approximates a discretized free space. The correspondence to free space becomes exact in the low-density limit. We focus on the crossover between the 1D and 2D geometry, therefore our Hubbard model corresponds to a rectangular lattice with $L \times W$ sites, where $1 \leq W < L$, but with the same lattice spacing $\alpha$ in both dimensions. We are using periodic boundary conditions in both directions, and thus our systems has the topology of a torus. The Hubbard Hamiltonian in momentum representation is

$$H = \sum_{\vec{k},s} \epsilon_{\vec{k}} c_{\vec{k}s}^\dagger c_{\vec{k}s} + \frac{U}{LW} \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3} c_{\vec{k}_1 \uparrow}^\dagger c_{\vec{k}_2 \downarrow}^\dagger c_{\vec{k}_3 \downarrow} c_{\vec{k}_1 \downarrow + \vec{k}_2 - \vec{k}_3 \uparrow},$$

(1)

where the operators $c_{\vec{k}s}^{(\dagger)}$ create (annihilate) a fermion with lattice momentum $\hbar \vec{k}$ and spin $s$. Wave vectors can take on values $\vec{k} = (k_x, k_y) = 2\pi (n_x/\alpha L, n_y/\alpha W)$, where $n_x, n_y$ are integers. The single-particle dispersion for the Hubbard model is given by

$$\epsilon_{\vec{k}} = 2t(2 - \cos(k_x \alpha) - \cos(k_y \alpha))$$

(2)

where $t$ is the hopping amplitude and $U < 0$ is the interaction parameter. In the low density regime, mostly the low-lying momentum states are occupied where the dispersion relation \[2\] is approximately parabolic. Thus the Hubbard model approximates a continuum Fermi gas.

Throughout this paper we present results obtained for a particle number of $N = 10$, with 5 fermions in each spin state, and a lattice length of $L = 21$, while the width $W$ varies from 1 to 11. Energies will be given in units of hopping amplitude $t$ and momenta in longitudinal lattice units $p_L = \frac{2\pi}{\alpha L}$.
III. FCIQMC

FCIQMC is a numerical method originally created in the context of strongly correlated electron systems and quantum chemistry. It can find ground states of fermionic many-body systems by expanding the many-body wave function in terms of Slater determinants

$$|\Psi\rangle = \sum_i C_i |D_i\rangle,$$

(3)

which in our case are of the form

$$|D\rangle = c_{k_1,s_1}^\dagger \ldots c_{k_N,s_N}^\dagger |\text{vac}\rangle.$$

(4)

FCIQMC then obtains the expansion coefficients $C_i$ by using a stochastic population dynamics approach to solve the imaginary-time Schrödinger equation. The automatic antisymmetrization of the wave function by expanding it in Slater determinants ensures that unlike Diffusion Monte-Carlo, FCIQMC always finds a fermionic wave function. FCIQMC’s capacity for overcoming the so-called “fermion sign problem”, which here manifests in fluctuations of the sign of each of the coefficients $C_i$ and which cannot be pre-determined, depends on the importance of annihilation events among the walkers in establishing the sign structure of the sampled wavefunction. When this effect is strong, the full FCIQMC method requires a number of walkers which scales with the size of the Hilbert space, making it impractical for large spaces.

To counter this, we use a range of modifications to FCIQMC, which facilitates calculations when the sign problem is strong. We make use of a similarity-transformed Hamiltonian which makes the many-body wave function more compact in Hilbert space [73]. We also use the initiator approximation [61], which can introduce a bias into the energy that disappears in the limit of large walker number. In order to control this undesirable bias, we first compare QMC results with exact results in the 1D case and then adjust the walker number until the initiator bias is eliminated. For the 2D systems, we successively increase the walker number with increasing $W$. Walker numbers used in this paper range from $N_W = 1 \times 10^6$ for weakly-interacting 1D chains to $N_W = 2 \times 10^8$ for 2D systems at $U/t = -5$. The most demanding computations were run on up to 400 processor cores using up to 2 Gigabyte memory per core.

IV. BETHE ANSATZ RESULTS

For a one-dimensional Hubbard chain ($W = 1$), the system is integrable and the Hamiltonian [1] can be diagonalized using the Bethe ansatz [74]. For a balanced Fermi system with $N$ fermions, energy and total momentum are given by

$$E = -2t \sum_{j=1}^{N} \cos(\kappa_j) + U(L - 2N),$$

(5)

$$P/P_0 = \sum_{j=1}^{N} \kappa_j \mod 2\pi,$$

(6)

with $N$ dimensionless quasi-momenta $\kappa_j$ which must be obtained, alongside $N/2$ rapidities $\Lambda_\alpha$, by solving the Lieb-Wu equations

$$\exp(i\kappa_j L) = \prod_{\alpha=1}^{N/2} \frac{\sin \kappa_j - \Lambda_\alpha + iU/4t}{\sin \kappa_j - \Lambda_\alpha - iU/4t},$$

(7)

$$\prod_{j=1}^{N} \frac{\sin \kappa_j - \Lambda_\beta + iU/4t}{\sin \kappa_j - \Lambda_\beta - iU/4t} = -\prod_{\alpha=1}^{N/2} \frac{\Lambda_\alpha - \Lambda_\beta + iU/2t}{\Lambda_\alpha - \Lambda_\beta - iU/2t}.$$ 

(8)

Solving the Lieb-Wu equations via root finding can be done with great accuracy and polynomial effort with particle number. The Bethe ansatz thus provides us with an exact reference for the one-dimensional Hubbard chain.

This allows us to compare QMC results with exact results to determine the parameter range where we can consider FCIQMC to be reliable in the sense that a possible initiator bias is smaller than the statistical uncertainty inherent in the Monte Carlo approach. In general, larger values of $|U/t|$ lead to stronger correlations in the many-body wave function, which then requires a larger number of Slater determinants to be accurately represented. Also, the fermionic sign problem becomes more
severe, which tends to increase the initiator bias in the calculated energy. In FIG. 1 we compare results obtained using the Bethe ansatz and FCIQMC results for a 1D chain (L = 21, W = 1). We see that for \(|U/t| < 5\) the agreement is very good. We therefore mainly use interaction strengths of \(|U/t| \leq 5\) in this paper, which covers the entire BEC-BCS crossover and typical values achievable in experiments \([59]\).

V. UMKLAPP POINTS

Figure 1 illustrates the characteristic shape of the yrast dispersion, which is concave downward resembling inverted parabolas in the intervals \(0 < P < P_0N/2\) and \(P_0N/2 < P < P_0N\), and with local minima at integer multiples of \(P_0N/2\). It can be understood by looking at the non-interacting case: To increase the total momentum of the system by a single unit of \(P_0\), first a fermion at the Fermi surface is excited. The resulting hole can then be filled by another fermion to increase the momentum again, and so forth, with the energy tracing the inverted parabolic part of the Hubbard lattice dispersion relation of Eq. (2). The first local minimum of the yrast spectrum, called the half-umklapp point, in our case \((N = 10)\) at \(P/P_0 = 5\) is reached when all particles of one spin component have each been boosted by \(P_0\). At that point, the Fermi surfaces of both components are shifted with respect to each other, but there are no holes in the Fermi seas of either spin species.

The full umklapp point at \(P/P_0 = 10\) is reached when both spin components, or all particles are boosted. In the continuum limit, where full Galilean invariance is restored, the excitation energy of the umklapp point is determined by the boost only and is independent of interactions, since the state is strictly a boosted ground state. In the lattice system, where Galilean invariance is broken, a weak interaction dependence at the umklapp points is nevertheless observed as seen in Fig. 1.

For a non-interacting 2D system, constructing the yrast dispersion from hole excitations leads to a different shape, which in the thermodynamic limit in an isotropic 2D system is linear. In our case, as is shown in FIG. 2 for \(W = 11\), due to finite-size effects in our mesoscopic system, the spectrum for \(U = 0\) has linear segments but is not perfectly linear. It is remarkable that for increasing interaction strength, the parabolic shape of the 1D spectrum with the umklapp points at \(P/P_0 = 5, 10\) is restored.

We can take a look at how the pairing in the system changes the characteristics of the umklapp points by calculating two-body correlation functions. It is possible to obtain the reduced two-body density matrix

\[
\Gamma_{s_1,s_2,s_3,s_4}(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4) = \langle \Psi_1| c_{\vec{k}_1,s_1}^\dagger c_{\vec{k}_2,s_2}^\dagger c_{\vec{k}_3,s_3} c_{\vec{k}_4,s_4} |\Psi_2\rangle
\]

(9)

from FCIQMC by simultaneously running two statistically independent QMC simulations with solutions \(\Psi_1, \Psi_2\), to avoid biases \([74]\). This is valuable even in the 1D case as obtaining the same quantity from the Bethe-ansatz solution is not feasible. To illustrate the BEC-BCS crossover, we show the opposite-spin pair correlation function \(g_{\uparrow\downarrow}(\vec{k}_1,\vec{k}_2) = \Gamma_{\uparrow\downarrow\uparrow\downarrow}(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\) for the ground state and half-umklapp point in the 1D case in FIG. 3.
Strong pair correlations with \( k_1 + k_2 = 0 \) clearly emerge as interaction strength is increased from \( U/t = -1 \) to \( U/t = -5 \). The \( P/P_0 = 5 \) half-umklapp point at weak interactions exhibits mostly the physics of a non-interacting system, with two Fermi seas displaced with respect to each other. This is in stark contrast to the situation at \( U/t = -5 \), where the correlation function is the same as for \( P = 0 \) but shifted in momentum space. The mere translation of the pair correlation function is consistent with interpreting the system as a superfluid of 5 bosonic pairs, where total momentum \( P/P_0 = 5 \) corresponds to a full umklapp (i.e. Galilean boost of the ground state) in contrast to the weakly-interacting Fermi gas, which only reaches a half umklapp point at this momentum.

The yrast excitation energy at the half umklapp point \( P_0 = P_0 N/2 \) and at the full umklapp point \( P_u = P_0 N \) are shown in Fig. 4. The lattice results can be compared to the expected excitation energies in an equivalent free-space system. The behavior of the umklapp points of an attractive 1D Fermi gas in free space has been studied using the Yang-Gaudin (YG) model [47]. There, the energy of the full umklapp point is independent of the interaction strength, as it represents simply a translation of the entire Fermi sea in momentum space. In the YG model this energy is given by \( E - E_0 = P_u^2/2Nm \), where \( N \) is the total particle number and \( P_u = P_0 N \) the full umklapp momentum. In units of the Hubbard model parameters, this excitation energy is \( E - E_0 = 40\pi^2t/L^2 \) and is depicted as the upper dashed horizontal line in Fig. 4 (a). The half-umklapp point however drops by factor of 2 from \( E - E_0 = P_h^2/2mN \) to \( E - E_0 = P_0^2/2mN \), as it changes from being the half-umklapp point of a system of \( N \) fermions to being the full umklapp point of a gas of \( N/2 \) bosons. This is shown as the two lower dashed horizontal lines in Fig. 4 (a), with energies \( E - E_0 = 20\pi^2t/L^2 \) and \( E - E_0 = 10\pi^2t/L^2 \).

For the non-interacting case we observe expected behavior with energy values slightly lower than the YG model. This is because the YG model uses a quadratic dispersion written in parameters of the Hubbard model as

\[
\epsilon_k^{YG} = 2\alpha^2 k^2, \tag{10}
\]

and \( \epsilon_k \leq \epsilon_k^{YG} \).

However, for finite interactions the energy values we calculate for the Hubbard model do not behave like for the YG model. In our system, lattice effects dominate once the interaction is strong enough. It is known that for \( U/t \rightarrow -\infty \), the asymptotic effective Hamiltonian of the Hubbard model corresponds to a bosonic system with a one-boson-per-site hard-core condition and repulsive next-nearest neighbor interactions [26]. The effective Hamiltonian also has a global pre-factor of \( U^2/t \), meaning that the entire spectrum has the same scaling in the asymptotic regime. For the (half-)umklapp points, the asymptotes \( 80P_0^2/m \times t^2/U \) and \( 20P_0^2/m \times t^2/U \) are presented in Fig. 4 (a) as the green and purple dashed lines, respectively. We see that finite-size effects are reduced as the umklapp energies approach these asymptotic lines.
VI. MAXIMA OF THE YRAST SPECTRUM

The point $P = P_h/2$ near the first local maximum of the yраст spectrum (such as at $P/P_0 = 2, 3$ in Fig. 2) is of particular interest as a point where in the 1D homogeneous case dark solitons appear [27, 47, 47] that are stationary with respect to background and with phase step $\pi$ across the soliton. Dark solitons in a Fermi superfluid are characterized by a localized density depression and a phase jump in the superfluid order parameter around this depression. In a system with periodic boundary conditions, this phase jump must be compensated by a phase gradient along the system, which corresponds to a constant counterflow velocity $v_{cf}$. In addition, the soliton can be associated with an inertial mass $m_I$, related to the curvature of the yраст dispersion. We extract these parameters from our calculated dispersions by fitting the quadratic function

$$E(P) = E(0) + v_{cf}(P - P_h/2) + \frac{1}{2m_I}(P - P_h/2)^2$$

around the first local maximum at momenta $P/P_0 = 1, 2, 3, 4$, where $P_h = NP_0/2 = 5P_0$.

The results for the inertial mass are shown in Fig. 5, where we only show data points for the parameters where the yраст dispersion closely resembles a parabolic shape. This would correspond to a regime where a superfluid is present and the particles are strongly paired. This is mostly the case for $W \leq 7$, where the system is still effectively one-dimensional and transverse momentum states are sparsely populated. For the larger and more 2D systems with $W = 7, 9$, we find that for $|U/t| = 1, 5$, a parabolic yраст spectrum reappears (see also Fig. 4). For the effective mass, there is an increase in magnitude by a factor of 2 as we increase the system size to $W = 11$. This indicates a further change to the properties of the system, likely a transition from a soliton state to a vortex pair. This scenario is closely related to the snaking instability of a planar dark soliton in a two-dimensional superfluid, where the soliton decays into pairs of oppositely charged vortices as the system becomes wide enough [11, 65, 70]. However, we cannot directly show a potential density depression caused by the soliton. The reason is that, unlike in mean-field theory, our technique provides the many-body wave function of a (translationally invariant) eigenstate of total momentum and thus a superposition of solitons at all possible positions. The real-space single-particle density we can calculate is flat. To map out the dark soliton as described in [77], we would need access to higher-order density matrices beyond the two-body density matrix. Therefore, it remains to be seen if the increase in inertial mass really corresponds to a soliton-vortex pair transition.

![Graph showing inertial mass vs. interaction strength](image)

**FIG. 5.** Inertial mass of the first yраст maximum vs. interaction strength. Unlike in free space, in the lattice, the inertial mass asymptotically approaches $-\infty$ linearly with the interaction strength $U/t$. In the 2D regime, where a parabolic yраст dispersion reappears for strong interactions, the inertial mass is larger by a factor of 2.

Instead, we investigate more closely the pair condensation, for which a relevant quantity is the pair Green’s function

$$G_p(l) = \langle \psi^\dagger_{j+1,\uparrow} \psi^\dagger_{j+1,\downarrow} \psi_{j,\downarrow} \psi_{j,\uparrow} \rangle,$$

where $\psi$ and $\psi^\dagger$ denote creation and annihilation operators, respectively, in position space. The Fourier transform of this Green’s function is the momentum-space pair density. For a system with a homogeneous density, it can be directly obtained from the momentum representation
of the two-body density matrix

\[ n_p(\vec{k}) = \sum_{\vec{k}_1, \vec{k}_2} \Gamma^{\uparrow \downarrow \uparrow \downarrow}(\vec{k}_1, \vec{k} - \vec{k}_1, \vec{k}_2, \vec{k} - \vec{k}_2). \]  

(13)

This quantity indicates whether Bose-Einstein condensation of pairs occurs. While we find evidence of Bose-Einstein condensation of pairs by a peak in the pair density that grows with increasing interaction strength for the ground state and umklapp point, the situation is more complex for general yrast states. In Fig. 6 we show the pair density for a 2D system with \(21 \times 11\) sites for interaction parameters \(U/t = -1\) and \(U/t = -5\), for the ground state and the \(P/P_0 = 2\) yrast state. For weak interactions, the structure of the pair density is determined mostly by the structure of the Fermi sea, or the noninteracting yrast state. For stronger interactions, the ground state exhibits one sharp peak at zero momentum indicating strong pairing correlations, as expected for crossover to a BEC of pairs. However, for \(P/P_0 = 2\), there are actually two peaks, for longitudinal momenta 0 and 2\(P_0\). Similar features appear in the smaller 2D and 1D systems.

We now show that this double-peak feature signifies the presence of fragmented condensation. Fragmentation occurs when during the transition to a Bose-Einstein condensate, more than one state becomes macroscopically occupied \cite{78}. In Fig. 6 the momentum states (0, 0) and (2\(P_0\), 0) dominate the pair density. For the 1D system, where obtaining the reduced density matrices is easier, we plot the pair densities of several momenta for the yrast state with \(P = 3P_0\) in Fig. 7 as a function of interaction strength. We see that in addition to \(P = 0\), the pair density at \(P = P_0\) strongly increases as well. Similarly, for other yrast states we see the same phenomenon, a strong signature of fragmented condensation. It is worth noting that the pair density with two peaks obtained here is similar to the case of an imbalanced Fermi gas, where Fermi surfaces of different size lead to FFLO pairing with non-zero total momentum and the signature is a two-peaked pair-density. This has been studied for 1D and 2D Hubbard models \cite{44,57,75,79,80}. Yrast states in our balanced system start with holes in one of the Fermi seas for weak interaction, which also leads to pairing with non-zero total momentum.

VII. CONCLUSIONS

In this paper, we have used the FCIQMC method to study the crossover from weakly interacting fermions to a condensate of bosonic pairs for yrast states in mesoscopic Fermi systems. With this method we can treat larger systems than are accessible to the previously used deterministic CI or exact diagonalization methods \cite{48,49} and can probe the full transition from a 1D chain not just to quasi-1D rings, but also to full 2D systems. We obtain energy spectra and reduced two-body density matrices for yrast states in the attractive Hubbard model in these geometries.

Comparisons with exact Bethe ansatz results in 1D show very good agreement and demonstrate that FCIQMC can accurately provide yrast states for mesoscopic systems with 10 fermions and \(21 \times W\) sites where \(W\) ranges from 1 to 11. We find that the shape of the yrast spectrum changes from the typical inverted parabolas in 1D to a quasi-linear spectrum in 2D. However, as interaction strength is increased, the parabolic dispersion including the half umklapp point is restored. While the quasi-linear spectrum is a consequence of the 2D geometry and the Pauli exclusion principle, with stronger interactions the exact shape of the non-interacting Fermi sea plays less of a role until we see the expected universal concave downward dispersion of a spinless superfluid. This indicates a transition to a fully paired Fermi superfluid.

We further find that mesoscopic effects can cause significant deviations for certain geometries from the general behavior of the umklapp energies, which otherwise does not differ much between 1D and 2D systems. Specifically we find that the half-umklapp excitation energy for a lattice of \(21 \times 11\) points increases with interaction strength at intermediate values of \(U/t\) contrary to the general trend displayed by all other systems under study. This originates in a rearrangement of the fermions in momentum space, where for this particular geometry, the half-umklapp point is a different configuration than the ground state with one spin component shifted in momen-
These pair densities of yrast states share some similarities. The momentum pairs becomes large for strong interactions. With zero total momentum, the amplitude of other total peaked pair densities appear, where in addition to pairing away from the umklapp points. We find that here, multi-pair of oppositely charged vortices is no longer stable and the yrast state is instead provided by pair of oppositely charged vortices.

The most striking feature of yrast states in the Hubbard model is revealed to be fragmented condensation, which occurs around the maxima of the yrast dispersion, is no longer stable and the yrast state is instead provided by pair of oppositely charged vortices. In the FFLO case, which occurs around the maxima of the yrast dispersion, the Fermi surfaces are shifted in momentum space. In addition, both yrast and FFLO states are related to solitons in the real space density.

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[1] DM Eagles, “Possible Pairing without Superconductivity at Low Carrier Concentrations in Bulk and Thin-Film Superconducting Semiconductors,” Phys. Rev. Lett. 53, 456, 1959.

[2] Anthony J Leggett, “Diatomic Molecules and Cooper pairs,” in Mod. Trends Theory Condens. Matter Lecture Notes in Physics, edited by Andrzej Pękalski and Jerzy A Przystawa (Springer Berlin Heidelberg, 1980) pp. 13–27.

[3] Wilhelm Zwerger, ed., The BCS — BEC Crossover and the Unitary Fermi Gas Lecture Notes in Physics, Vol. 836 (Springer Berlin / Heidelberg, Berlin, Heidelberg, 2012) p. 532, arXiv:1008.3933.

[4] Jesper Levinsen and Meera M. Parish, “Strongly interacting two-dimensional Fermi gases,” in Ann. Rev. Cold Atoms Mol. (WORLD SCIENTIFIC, 2015) pp. 1–75.

[5] Stefano Giorgini and Sandro Stringari, “Theory of ultracold atomic Fermi gases,” Rev. Mod. Phys. 80, 1215–1274 (2008), arXiv:0706.3360.

[6] Meera M. Parish, “The BCS-BEC Crossover,” in Quantum Gas Exp., edited by Päivi Törmä and Klaus Sengstock (Imperial College Press, 2014) pp. 179–197, arXiv:1402.5171.

[7] C. A. Regal, M. Greiner, and D. S. Jin, “Observation of Resonance Condensation of Fermionic Atom Pairs,” Phys. Rev. Lett. 92, 040403 (2004) arXiv:0401554 [cond-mat].

[8] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, A. J. Kerman, and W. Ketterle, “Condensation of Pairs of Fermionic Atoms near a Feshbach Resonance,” Phys. Rev. Lett. 92, 120403 (2004).

[9] C. Chin, M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, J. Hecker Denschlag, and R. Grimm, “Observation of the Pairing Gap in a Strongly Interacting Fermi Gas,” Science 305, 1128–1130 (2004) arXiv:0405632 [cond-mat].

[10] T. Bourdel, L. Khaykovich, J. Cubizolles, J. Zhang, F. Chevy, M. Teichmann, L. Tarruell, S. J. J. M. F. Kokkelmans, and C. Salomon, “Experimental Study of the BEC-BCS Crossover Region in Lithium 6,” Phys. Rev. Lett. 93, 050401 (2004) arXiv:0403091 [cond-mat].

[11] J. Kinast, S. L. Hemmer, M. E. Gehm, A. Turlapov, and J. E. Thomas, “Evidence for Superfluidity in a Resonantly Interacting Fermi Gas,” Phys. Rev. Lett. 92, 150402 (2004).

[12] Wolfgang Ketterle and Martin W Zwierlein, “Making, probing and understanding ultracold Fermi gases,” Riv. del Nuovo Cim. 31, 247 (2008) arXiv:0801.2500.

[13] M. J. H. Ku, A. T. Sommer, L. W. Cheuk, and M. W. Zwierlein, “Revealing the Superfluid Lambda Transition in the Universal Thermodynamics of a Unitary Fermi Gas,” Science 335, 563–567 (2012).

[14] C. Carey, S. Hoinka, M. G. Lingham, P. Dyke, C. C. N. Kuhn, H. Hu, and C. J. Vale, “Contact and Sum Rules in a Near-Uniform Fermi Gas at Unitarity,” Phys. Rev. Lett. 122, 203401 (2019), arXiv:1902.07853.

[15] Biswaroop Mukherjee, Parth B. Patel, Zhenjie Yan, Richard J. Fletcher, Julian Struck, and Martin W. Zwierlein, “Spectral Response and Contact of the Unitary Fermi Gas,” Phys. Rev. Lett. 122, 203402 (2019), arXiv:1902.08548.

[16] Waseem S Bakr, Jonathon I Gillen, Amy Peng, Simon Folling, and Markus Greiner, “A quantum gas microscope for detecting single atoms in a Hubbard-regime optical lattice,” Nature 462, 74–77 (2009).

[17] Lawrence W Cheuk, Matthew A Nichols, Melih Olan, Thomas Gersdorf, Vinay V Ramasesh, Waseem S Bakr, Thomas Long, and Martin W Zwierlein, “Quantum-Gas Microscope for Fermionic Atoms,” Phys. Rev. Lett. 114, 193001 (2015).

[18] Elmar Haller, James Hudson, Andrew Kelly, Dylan A.
Cotta, Bruno Peudecerf, Graham D. Bruce, and Stefan Kuhr, “Single-atom imaging of fermions in a quantum-gas microscope,” Nat. Phys. 11, 738–742 (2015).

[19] Peter T. Brown, Elmer Guardado-Sanchez, Benjamin M. Spar, Edwin W. Huang, Thomas P. Devereaux, and Waseem S. Bakr, “Angle-resolved photoemission spectroscopy of a Fermi–Hubbard system,” Nat. Phys. 16, 26–31 (2020), arXiv:1903.05678.

[20] T. Grünzweig, A. Hilliard, M. McGovern, and M. F. Andersen, “Near-deterministic preparation of a single atom in an optical microtrap,” Nat. Phys. 6, 951–954 (2010).

[21] P. Serwane, G. Zürn, T. Lompe, T. B. Ottenstein, A. N. Wenz, and S. Jochim, “Deterministic preparation of a tunable few-fermion system,” Science 332, 336–338 (2011).

[22] A. Wenz, G. Zürn, S. Murmann, I. Bronzov, T. Lompe, and S. Jochim, “From Few to Many: Observing the Formation of a Fermi Sea One Atom at a Time,” Science 342, 457–460 (2013), arXiv:1307.3443v2.

[23] L. A. Reynolds, E. Schwab, U. Ebling, M. Weyland, J. Brand, and M. F. Andersen, “Direct Measurements of Collisional Dynamics in Cold Atom Triads,” Phys. Rev. Lett. 124, 073401 (2020), arXiv:2001.05141.

[24] P. P. Kulish, S. V. Manakov, and L. D. Faddeev, “Comparison of the exact quantum and quasiclassical results for a nonlinear Schrödinger equation,” Theor. Math. Phys. 28, 615–620 (1976).

[25] Rina Kanamoto, Lincoln D. Carr, and Masahito Ueda, “Topological Winding and Unwinding in Metastable Bose-Einstein Condensates,” Phys. Rev. Lett. 100, 060401 (2008).

[26] R. Kanamoto, L. D. Carr, and M. Ueda, “Metastable quantum phase transitions in a periodic one-dimensional Bose gas. II. Many-body theory,” Phys. Rev. A 81, 023625 (2010), arXiv:0910.2805.

[27] A. D. Jackson, J. Smyrnakis, M. Magiropoulos, and G. M. Kavoulakis, “Solitary waves and yrast states in bose-einstein condensed gases of atoms,” EPL (Europhysics Letters) 95, 30002 (2011).

[28] Oleksandr Fialko, Marie-Corail Delattre, Joachim Brand, and Andrey R. Kolovsky, “Nucleation in finite topological systems during continuous metastable quantum phase transitions,” Phys. Rev. Lett. 108, 250402 (2012).

[29] Jun Sato, Rina Kanamoto, Eriko Kaminishi, and Tetsuo Deguchi, “Exact relaxation dynamics of a localized many-body state in the 1D Bose gas,” Phys. Rev. Lett. 108, 110401 (2012), arXiv:1112.4244.

[30] Andrzej Syrwid and Krzysztof Sacha, “Lieb-Liniger model: Emergence of dark solitons in the course of measurements of particle positions,” Phys. Rev. A 92, 032110 (2015), arXiv:1505.06586.

[31] Sophie S. Shamailov and Joachim Brand, “Quantum dark solitons in the one-dimensional bose gas,” Phys. Rev. A 99, 043632 (2019).

[32] Toshio Tsuzuki, “Nonlinear waves in the Pitaevskii-Gross equation,” J. Low Temp. Phys. 4, 441 (1971).

[33] Tarik Yefsah, Ariel T Sommer, Mark J H Ku, Lawrence W. Cheuk, Wenjie Ji, Waseem S Bakr, and Martin W Zwierlein, “Heavy solitons in a fermionic superfluid,” Nature 499, 426–30 (2013), arXiv:1302.4736.

[34] Mark J. H. Ku, Wenjie Ji, Biswaroop Mukherjee, Elmer Guardado-Sanchez, Lawrence W. Cheuk, Tarik Yefsah, and Martin W Zwierlein, “Motion of a Solitonic Vortex in the BEC-BCS Crossover,” Phys. Rev. Lett. 113, 065301 (2014), arXiv:1402.7052.

[35] Mark J. H. Ku, Biswaroop Mukherjee, Tarik Yefsah, and Martin W Zwierlein, “Cascade of Solitonic Excitations in a Superfluid Fermi gas: From Planar Solitons to Vortex Rings and Lines,” Phys. Rev. Lett. 116, 045304 (2016), arXiv:1507.01047.

[36] Mauro Antezza, Franco Dalfovo, Lev Pitaevskii, and Sandro Stringari, “Dark solitons in a superfluid Fermi gas,” Phys. Rev. A 76, 043610 (2007), arXiv:0706.0061.

[37] Renyuan Liao and Joachim Brand, “Traveling dark solitons in superfluid Fermi gases,” Phys. Rev. A 83, 041604(R) (2011).

[38] R. Scott, F. Dalfovo, L. Pitaevskii, and S. Stringari, “Dynamics of Dark Solitons in a Trapped Superfluid Fermi Gas,” Phys. Rev. Lett. 106, 185301 (2011).

[39] Andrea Spuntarelli, Lincoln D Carr, Pierbiagio Pieri, and Giancarlo C Strinati, “Gray solitons in a strongly interacting superfluid Fermi gas,” New J. Phys. 13, 035010 (2011).

[40] R. G. Scott, F. Dalfovo, L. P. Pitaevskii, S. Stringari, O. Fialko, R. Liao, and J. Brand, “The decay and collisions of dark solitons in superfluid Fermi gases,” New J. Phys. 14, 023044 (2012), arXiv:1109.6444.

[41] A. Cetoli, J. Brand, R. G. Scott, F. Dalfovo, and L. P. Pitaevskii, “Snake instability of dark solitons in fermionic superfluids,” Phys. Rev. A 88, 043630 (2013), arXiv:1307.3717.

[42] Dmitry E. Efimkin and Victor Galitski, “Moving solitons in a one-dimensional fermionic superfluid,” Phys. Rev. A 91, 023616 (2015), arXiv:1408.6511.

[43] Nobukatsu Yoshida and S.-K. Yip, “Larkin-Ovchinnikov state in resonant Fermi gas,” Phys. Rev. A 75, 063601 (2007).

[44] Roman M. Lutchyn, Maxim Dzero, and Victor M. Yakovenko, “Spectroscopy of the soliton lattice formation in quasi-one-dimensional fermionic superfluids with population imbalance,” Phys. Rev. A 84, 033609 (2011).

[45] Peter Fulde and Richard A. Ferrell. “Superconductivity in a Strong Spin-Exchange Field,” Phys. Rev. 135, A550–A563 (1964).

[46] A.I. Larkin and Yu.N. Ovchinnikov, “Nonuniform state of superconductors,” Sov. Phys. JETP 20, 762 (1965).

[47] Sophie S. Shamailov and Joachim Brand, “Dark-soliton-like excitations in the Yang–Gaudin gas of attractively interacting fermions,” New Journal of Physics 18, 075004 (2016).

[48] S. Vieffers, P. Koskinen, P. Singha Deo, and M. Manninen, “Quantum rings for beginners: energy spectra and persistent currents,” Phys. E Low-dimensional Syst. Nanostructures 21, 1–35 (2004), arXiv:0310064 [cond-mat].

[49] M. Manninen, S. Vieffers, and S. M. Reimann, “Quantum rings for beginners II: Bosons versus fermions,” Phys. E Low-dimensional Syst. Nanostructures 46, 119–132 (2012).

[50] Vladimir M. Fomin, ed., Physics of Quantum Rings 2nd ed., NanoScience and Technology (Springer International Publishing, Cham, 2018) p. 585.

[51] Matthias Troyer and Uwe-Jens Wiese, “Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations,” Phys. Rev. Lett. 94, 170201 (2005), arXiv:0408370 [cond-mat].

[52] Congjun Wu and Shou-Cheng Zhang, “Sufficient condi-
tion for absence of the sign problem in the fermionic quantum Monte Carlo algorithm,” Phys. Rev. B 71, 155115 (2005).

[53] W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal, “Quantum Monte Carlo simulations of solids,” Rev. Mod. Phys. 73, 33–83 (2001).

[54] J. Carlson, Stefano Gandolfi, Kevin E. Schmidt, and Shiwei Zhang, “Auxiliary-field quantum Monte Carlo method for strongly paired fermions,” Phys. Rev. A 84, 061602 (2011).

[55] Mario Motta, Shiwei Zhang, and Garnet Kin-Lic Chan, “Hamiltonian symmetries in auxiliary-field quantum Monte Carlo calculations for electronic structure,” Phys. Rev. B 100, 045127 (2019).

[56] C. N. Varney, C.-R. Lee, Z. J. Bai, S. Chiesa, M. Jarrell, and A. Alavi, “Towards an exact description of electronic convergence in full configuration interaction quantum Monte Carlo,” J. Chem. Theory Comput. 14, 173–177 (2018). arXiv:1705.02039.

[57] M. J. Wolak, V. G. Rousseau, C. Miniatura, B. Grémaud, R. T. Scalettar, and G. G. Batrouni, “Finite-temperature quantum Monte Carlo study of the one-dimensional polarized fermi gas,” Phys. Rev. A 82, 013614 (2010).

[58] M. J. Wolak, B. Grémaud, R. T. Scalettar, and G. G. Batrouni, “Pairing in a two-dimensional fermi gas with population imbalance,” Phys. Rev. A 86, 023630 (2012).

[59] Debayan Mitra, Peter T. Brown, Elmer Guardado-Sanchez, Stanimir K. Kondov, Trithep Devakul, David A. Huse, Peter Schauf, and Waseem S. Bakr, “Quantum gas microscopy of an attractive Fermi–Hubbard system,” Nat. Phys. 14, 173–177 (2018). arXiv:1705.02039.

[60] George H. Booth, Alex J. W. Thom, and Ali Alavi, “Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in slater determinant space,” The Journal of Chemical Physics 131, 054106 (2009). https://aip.scitation.org/doi/pdf/10.1063/1.3193710.

[61] Deidre Cleland, George H. Booth, and Ali Alavi, “Communications: Survival of the fittest: Accelerating convergence in full configuration-interaction quantum Monte Carlo,” The Journal of Chemical Physics 132, 041103 (2010). https://doi.org/10.1063/1.3302277.

[62] George H Booth, Andreas Grüneis, Georg Kresse, and Ali Alavi, “Towards an exact description of electronic wavefunctions in real solids,” Nature 493, 365–70 (2013).

[63] Deidre Cleland, George H Booth, Catherine Overy, and Ali Alavi, “Taming the first-row diatomics: A full configuration interaction quantum Monte Carlo study,” J. Chem. Theory Comput. 8, 4138–4152 (2012).

[64] Péter Jeszenszki, Ulrich Ebling, Hongjun Luo, Ali Alavi, and Joachim Brand, “Eliminating the wavefunction singularity for ultracold atoms by a similarity transformation,” Phys. Rev. Res. 2, 043270 (2020). arXiv:2002.05987.

[65] Mingrui Yang, Elke Pahl, and Joachim Brand, “Improved walker population control for full configuration interaction quantum Monte Carlo,” J. Chem. Phys. 153, 174103 (2020). arXiv:2008.01927.

[66] J. S. Spencer, N. S. Blunt, and W. M. C. Foulkes, “The sign problem and population dynamics in the full configuration interaction quantum Monte Carlo method,” The Journal of Chemical Physics 136, 054110 (2012). https://doi.org/10.1063/1.3681396.

[67] Joachim Brand and William P Reinhardt, “Generating ring currents, solitons and svortices by stirring a Bose-Einstein condensate in a toroidal trap,” J. Phys. B At. Mol. Opt. Phys. 34, L113–L119 (2001).

[68] Joachim Brand and William P. Reinhardt, “Solitonic vortices and the fundamental modes of the "snake instability": Possibility of observation in the gaseous Bose-Einstein condensate,” Phys. Rev. A 65, 043612 (2002).

[69] A. Muñoz Mateo and J. Brand, “Chladni Solitons and the Onset of the Snaking Instability for Dark Solitons in Confined Superfluids,” Phys. Rev. Lett. 113, 255302 (2014). arXiv:1408.0947.

[70] W. Van Alphen, H. Takeuchi, and J. Tempere, “Crossover between snake instability and josephson instability of dark solitons in superfluid fermi gases,” Phys. Rev. A 100, 023628 (2019).

[71] A. Muñoz Mateo and J. Brand, “Stability and dispersion relations of three-dimensional solitary waves in trapped Bose-Einstein condensates,” New J. Phys. 17, 125013 (2015). arXiv:1510.01465.

[72] L. A. Tolka and J. Brand, “Asymptotically solvable model for a solitonic vortex in a compressible superfluid,” New J. Phys. 19, 023029 (2017). arXiv:1608.08701.

[73] Werner Dobrzutz, Hongjun Luo, and Ali Alavi, “Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via nonunitary similarity transformations,” Phys. Rev. B 99, 075119 (2019).

[74] Elliott H. Lieb and F. Y. Wu, “The one-dimensional hubbard model: a reminiscence,” Physica A: Statistical Mechanics and its Applications 321, 1–27 (2003) statphys-Taiwan-2002: Lattice Models and Complex Systems.

[75] Catherine Overy, George H. Booth, N. S. Blunt, James J. Shepherd, Deidre Cleland, and Ali Alavi, “Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo,” J. Chem. Phys. 141, 244117 (2014).

[76] A Teubel, E Kolley, and W Kolley, “On a unified canonical transformation of the large-negative-(positive-)u hubbard model,” Journal of Physics A: Mathematical and General 23, L837–L840 (1990).

[77] Andrzej Syrwid, Dominique Delande, and Krzysztof Sacha, “Emergence of dark soliton signatures in a one-dimensional unpolarized attractive fermi gas on a ring,” Phys. Rev. A 98, 023616 (2018).

[78] Erich J. Mueller, Tin-Lun Ho, Masahito Ueda, and Gordon Baym, “Fragmentation of bose-einstein condensates,” Phys. Rev. A 74, 033612 (2006).

[79] Song Cheng, Yuzhu Jiang, Yi-Cong Yu, Murray T. Batchelor, and Xi-Wen Guan, “Asymptotic correlation functions and ffo signature for the one-dimensional attractive Hubbard model,” Nuclear Physics B 929, 353–376 (2018).

[80] Song Cheng, Yi-Cong Yu, M. T. Batchelor, and Xi-Wen Guan, “Fulde-ferrlarkin-ovchinnikov correlation and free fluids in the one-dimensional attractive hubbard model,” Phys. Rev. B 97, 121111 (2018).