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Harmonically trapped fermions in two dimensions: Ground-state energy and contact of SU(2) and SU(4) systems via a nonuniform lattice Monte Carlo method

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We study harmonically trapped, unpolarized fermion systems with attractive interactions in two spatial dimensions with spin degeneracies $N_f = 2$ and 4 and $N/N_f = 1, 3, 5,$ and 7 particles per flavor. We carry out our calculations using our recently proposed quantum Monte Carlo method on a nonuniform lattice. We report on the ground-state energy and contact for a range of couplings, as determined by the binding energy of the two-body system, and show explicitly how the physics of the N_f-body sector dominates as the coupling is increased.

I. INTRODUCTION

In the past year, there have been multiple reports on experiments with ultracold fermionic atoms in constrained, quasi-two-dimensional optical traps. For instance, the Berezinskii-Kosterlitz-Thouless superfluid transition [1] was observed in Refs. [2,3], and the finite-temperature thermodynamics was studied in Refs. [4,5]. The first realization of two-dimensional (2D) systems was in fact reported only a few years ago in [6,7], and since then multiple efforts followed, such as radio frequency spectroscopy [8,9], studies of dimensional crossover [10,11], polarons [12], density distribution [13], viscosity [14], Tan's contact [15], ground-state pressure [16], and polarized systems [17] (see also [18,19]).

Experiments continue to move forward at an exciting pace, and consistent advances are seen on the theory side as well. Early analytic studies considered pairing in the 2D Bose-Einstein condensation and Bardeen-Cooper-Schrieffer crossover at the mean-field level [20–22]. The ground-state equation of state was obtained in an *ab initio* fashion only in 2011, in Ref. [23]. Reference [24] followed up with a more detailed first-principles study of the ground state where the pressure, contact, pairing properties, and condensate fraction were determined. The thermal equation of state was first computed in Ref. [25] in the virial expansion, and in the Luttinger-Ward approach in Ref. [26]. Pair correlations were investigated in Ref. [27] in dilute, high-temperature regimes using the virial expansion, and in Ref. [28], which also analyzed Tan's contact. The work of Refs. [29–31] studied collective modes, while the shear viscosity and spin diffusion were calculated in Ref. [32]. Finite-temperature quantum Monte Carlo calculations characterized the density, pressure, compressibility, and contact more recently in Ref. [33], and a comparison between theory and experiment was carried out in [34].

The present work aims to complement some of the above computational studies by reporting our Monte Carlo calculations of the ground-state energy and contact of 2D fermions in a harmonic oscillator (HO) trap. Our calculations were performed in a nonuniform lattice, a technique put forward in Ref. [35]. We study spin degeneracies $N_f = 2$ and 4 and unpolarized systems of N particles for $N/N_f = 1,3,5,7$. In this first paper we do not study higher values of N_f,

although such calculations are certainly feasible with the same methods. This is particularly interesting given the progress in the experimental realization of SU(N_f)-symmetric systems in the last few years, in particular in the presence of optical lattices [36]. Moreover, experiments involving a small number of atoms have been achieved as well [37], and for those experiments, if ever carried out in 2D, the present work represents a prediction (see [38] for a recent review).

II. HAMILTONIAN AND MANY-BODY METHOD

As mentioned above, we focus here on a 2D system of N_f fermion species, attractively interacting via pairwise interactions. The full Hamiltonian in second quantization form is

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{int}}, \tag{1}$$

where

$$\hat{T} = \sum_{s=1}^{N_f} \int d^2p \left(\frac{\mathbf{p}^2}{2m} \right) \hat{n}_s(\mathbf{p}) \tag{2}$$

is the kinetic energy operator,

$$\hat{V}_{\text{ext}} = \sum_{s=1}^{N_f} \int d^2x \left(\frac{1}{2} m\omega^2 \mathbf{x}^2 \right) \hat{n}_s(\mathbf{x}) \tag{3}$$

is the external potential energy operator, and

$$\hat{V}_{\text{int}} = -\frac{g}{2} \sum_{s \neq s'} \int d^2x \, \hat{n}_s(\mathbf{x})\hat{n}_{s'}(\mathbf{x}) \tag{4}$$

is the two-body interaction operator. In the above equations, $\hat{n}_s(\mathbf{p})$ and $\hat{n}_s(\mathbf{x})$ are, respectively, the particle-density operators in coordinate and momentum space for species s, and we have included an overall factor of $1/2$ to avoid overcounting in the flavor sum.

As in Ref. [35], but now in 2D, we place the system in a discretized space of $N_x \times N_x$ points using the Gauss-Hermite lattice $\{x_i, y_j\}$ and weights $\{w_i, w_j\}$ of Gaussian quadratures in each direction to define such a lattice [39]. The discretized

form of the interaction then becomes

$$\hat{V}_{\text{int}} = -\frac{g}{2} \sum_{s \neq s'} \sum_{i,j=1}^{N_x} w_i w_j e^{x_i^2 + y_j^2} \hat{n}_{s,(i,j)} \hat{n}_{s',(i,j)}, \qquad (5)$$

where $\hat{n}_{s,(i,j)}$ is the lattice density operator for spin s at position (i,j). Thus, we obtain a position-dependent coupling constant $g(x_i, y_j) = g w_i w_j e^{x_i^2 + y_j^2}$.

Following the usual path of the lattice Monte Carlo formalism, we then approximate the Boltzmann weight using a symmetric Suzuki-Trotter decomposition:

$$e^{-\tau \hat{H}} = e^{-\tau/2(\hat{T} + \hat{V}_{\text{ext}})} e^{-\tau \hat{V}_{\text{int}}} e^{-\tau/2(\hat{T} + \hat{V}_{\text{ext}})} + O(\tau^3), \qquad (6)$$

for some small temporal discretization parameter τ (which below we take to be $\tau = 0.05$ in lattice units). This discretization of imaginary time results in a temporal lattice of extent N_τ, which we also refer to below in terms of $\beta = \tau N_\tau$ and in dimensionless form as $\beta \omega$. A Hubbard-Stratonovich transformation [40] of the interaction factor is then used to

represent the interaction using an auxiliary field (see, e.g., [41]), which results in a field-integral form of the left-hand side of Eq. (6). We use that form combined with the power-projection method [42] to obtain ground-state properties of the system, using a Slater determinant of HO single-particle orbitals as a trial wave function.

As in our previous work, we tune the system to specific physical points by way of the 2D scattering length a_0 between any two *different* species. We present a_0 everywhere in units of the HO length scale a_{HO} (which is 1 in our units, such that $\omega = 1/a_{\text{HO}}^2 = 1$). To this end, we computed the ground-state energy E_{GS} of the two-body problem and matched it to that of the continuum solution, for which the relationship between E_{GS} and the scattering length is well known (see, e.g., Ref. [43]). We used this renormalization procedure for each lattice size, and then proceeded to higher particle numbers using the coupling thus determined. To illustrate the success of the procedure, we show the results for the unpolarized spin-1/2 six-body problem in Fig. 1 for several lattice sizes. As can be appreciated in that figure, the finite-size effects are vanishingly small for $N_f = 2$. The same holds for $N_f = 4$, but only in the weakly coupled regime $2a_{\text{HO}}/a_0 < 0.6$. To account for these effects in the strong-coupling regime of the $N_f = 4$ case, we used $N_x = 40$.

III. ANALYSIS AND RESULTS

In this section we present our results for the energy per particle and Tan's contact. In all of our tests, as illustrated in the previous section, the lattice-size effects were very small. However, increasing N_f effectively enhances the attractive interaction, such that bound states become even more deeply bound, which in turn amplifies lattice-spacing effects (see also Ref. [44]). For this reason, we do not consider $N_f > 4$ in this work. As a compromise with the computational cost of running the calculations, we chose to fix $N_x = 10$ for $N_f = 2$ and $N_x = 40$ for $N_f = 4$, and explore a range of values of N/N_f. To minimize statistical effects, we took 10^4 decorrelated samples of the auxiliary field σ, which results in a statistical uncertainty of order 1%.

A. Ground-state energy

In Fig. 2 we show our results for the ground-state energy of systems with $N_f = 2$ and 4. For each flavor number, we studied systems with $N/N_f = 1, 3, 5$, and 7 particles per flavor. In all cases, as evident from the figures, the energy *per particle* monotonically increases when the particle number is increased, which seems to indicate that no new N-body bound states appear for $N > N_f$ (i.e., other than the one at $N/N_f = 1$). Likewise, in all cases we find that, at fixed N_f, the energy per particle heals to the energy of the $N/N_f = 1$ case, i.e., it is dominated by the N_f-body bound-state contribution. To see this in more detail, we show the energy again in Fig. 3, where we have subtracted the energy per particle of the $N/N_f = 1$ case from that of the $N/N_f = 3, 5, 7$ cases. At strong coupling that energy difference falls below the energy per particle of the system (somewhat more noisily in the $N_f = 4$ case than for $N_f = 2$), which shows that the N_f-body bound-state energy dominates the picture. While qualitatively
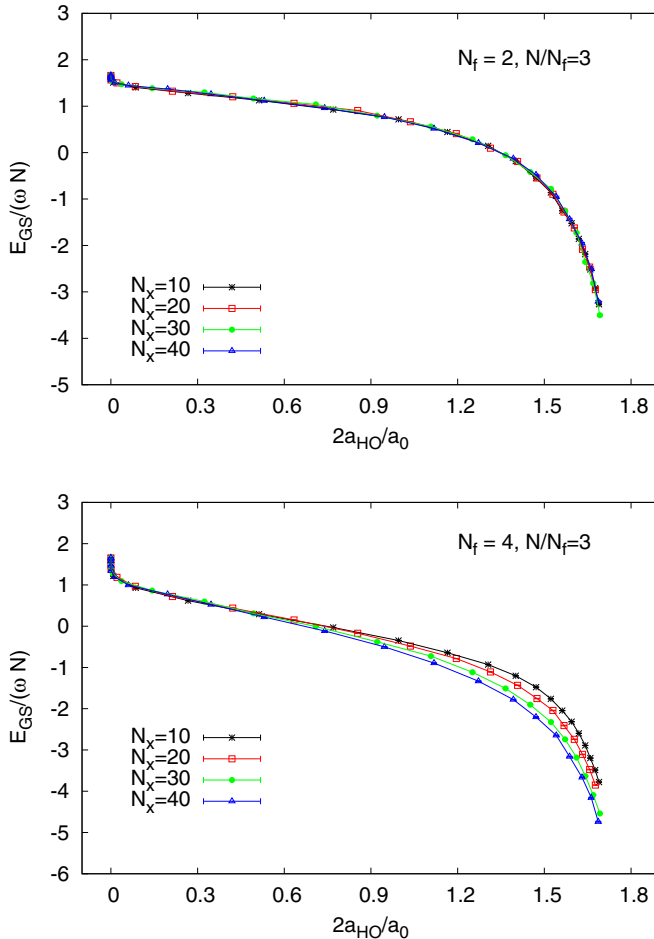

FIG. 1. Ground-state energy per particle of six spin-1/2 fermions (top figure) and 12 spin-3/2 fermions (bottom figure) harmonically trapped in 2D as a function of the coupling strength $2a_{\text{HO}}/a_0$ for four different lattice sizes $N_x = 10, 20, 30, 40$. The error bars reflect the statistical uncertainty. The exact result at $2a_{\text{HO}}/a_0 = 0$, i.e., for the noninteracting case, for spin-1/2 is $E/(\hbar \omega N) = 5/3$, but the approach is logarithmic, which explains the peaklike structure at very weak coupling (see figures below).
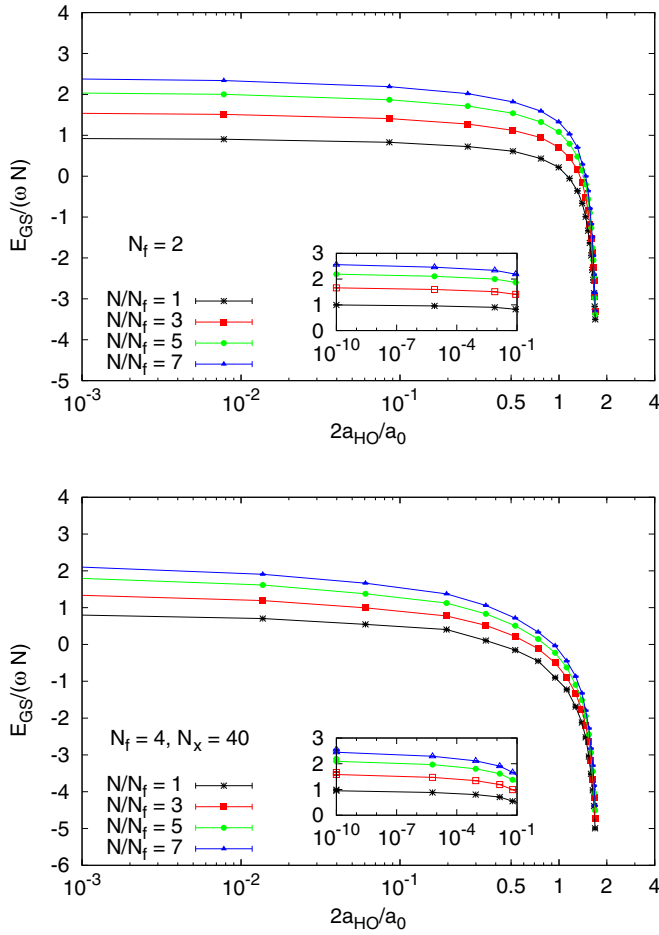
FIG. 2. Ground-state energy of $N_f = 2$ (top) and 4 (bottom) species of harmonically trapped fermions in 2D as a function of the coupling strength $2a_{HO}/a_0$, for particle numbers $N/N_f = 1,3,5,7$ (from bottom to top). The error bars reflect the statistical uncertainty. The inset shows the (logarithmic) approach to the noninteracting limit. For $N_f = 2$ the exact values of E_{GS}/N in the noninteracting limit are (from bottom to top) 1, 5/3, 12/5, and 3.
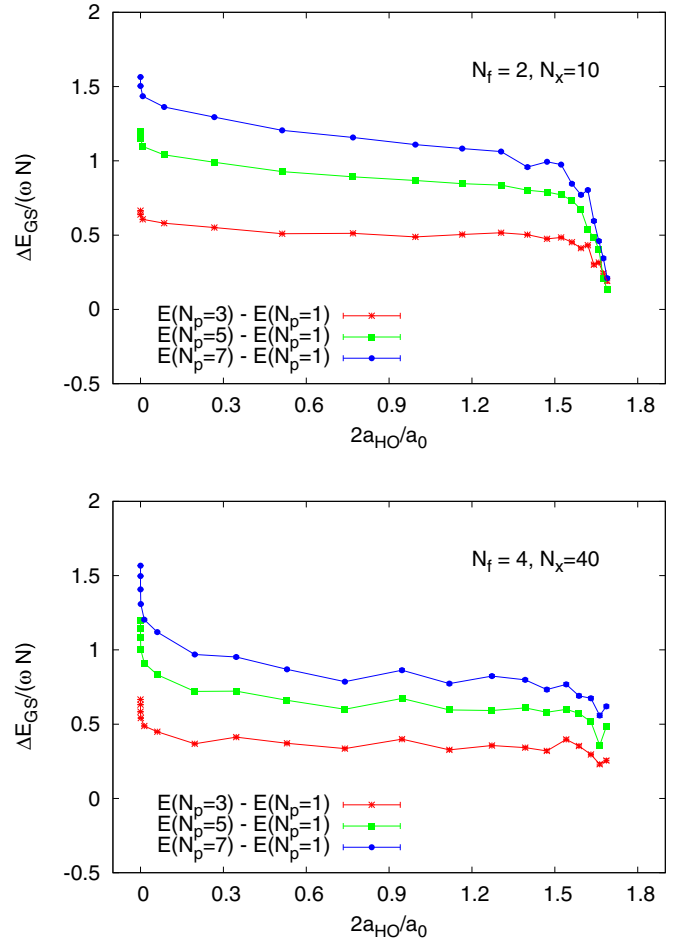

FIG. 3. Energy per particle difference, taking $N/N_f = 1$ as a reference, for $N_f = 2$ and $N_f = 4$ species of harmonically trapped fermions in 2D as a function of the coupling strength $2a_{HO}/a_0$, and for particle numbers $N/N_f = 3,5,7$ (from bottom to top).

this is not an unexpected result, our calculations show it in a quantitatively clear fashion. Furthermore, this suggests that, for each N_f, no new N-body bound states appear beyond the $N = N_f$ case.

B. Tan's contact

Besides the ground-state energy, one of the most interesting quantities in many-body systems with short-range interactions is Tan's contact [45,46]. This quantity is thermodynamically conjugate to the renormalized coupling, as shown by several authors [47–49]. Indeed, one way to find it is to determine the change in the energy with the scattering length (which is often referred to as the "adiabatic theorem"). Early on, it was shown by Tan that the contact determines the high-momentum tail of the momentum distribution, and this was soon afterwards associated with the operator-product expansion of high-energy physics [50], and since then several authors have derived exact results in the form of sum rules for response functions and high-energy or short-distance behavior of correlation functions.

Because our calculations used a contact interaction, the determination of the contact is essentially given by differentiation of the ground-state energy with respect to the bare coupling. Indeed, according to the adiabatic theorem in 2D [48,51],

$$C = 2\pi \frac{\partial E_{GS}}{\partial \ln(a_0/a_{HO})} = 2\pi \langle \hat{V} \rangle \frac{\partial \ln g}{\partial \ln(a_0/a_{HO})}, \quad (7)$$

i.e., computing C reduces to finding the ground-state expectation value of the potential energy operator $\hat{V}$ in the many-body problem, as the remaining factor is entirely due to two-body physics. The same is true in the present ground-state approach.

Our results for C are shown in Fig. 4, where we compare the contact per particle C/N for $N_f = 2$ and 4 with the two-body result. While at weak couplings the $N_f = 4$ result is above the two-body answer, we find that both $N_f = 2$ and 4 appear to approach that answer at strong coupling. This indicates that, in absence of a better guess, one may safely use the two-body contact in the many-body problem at strong coupling, even as N_f is increased.
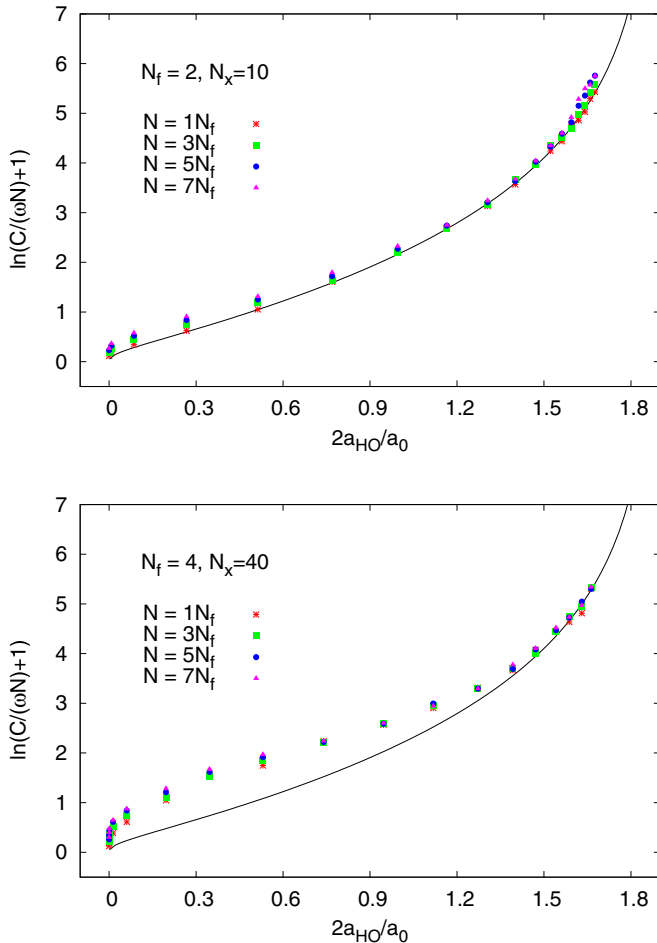
FIG. 4. Ground-state contact per particle of $N_f = 2$ (top) and 4 (bottom) species of harmonically trapped fermions in 2D, in units of the HO frequency ω, as a function of the coupling strength $2a_{HO}/a_0$, for particle numbers $N/N_f = 1,3,5,7$. The solid line shows, as a reference, the two-body result for $N_f = 2$.

IV. SUMMARY AND CONCLUSIONS

We used our recently proposed method of nonuniform lattice quantum Monte Carlo to analyze the behavior of few- to many-body systems of fermions in a two-dimensional harmonic trap. We explored systems of $N_f = 2$ and 4 flavors and up to $N/N_f = 7$ particles per flavor and focused on two experimentally measurable quantities: the ground-state energy and Tan's contact. While higher values of N_f are possible, we have determined that finite-size effects can be sizable when N_f is increased (although they appear to be vanishingly small for the systems studied here). Previous work (e.g., [25] or [52]) studied the exact spectrum of the three-body problem in 2D; our work complements and extends those approaches (though restricting ourselves to the ground state only). As harmonically trapped 2D systems are under intense experimental study at the moment, calculations of these basic quantities are timely [38]. Future 2D experiments with large-N_f atoms can be expected, for which our results are a prediction [36].

We find that the ground-state energy per particle shows no qualitative difference for $N_f = 2$ and 4: it increases monotonically for all the couplings we studied when the particle number per flavor N/N_f is increased. On the other hand, at fixed N/N_f, increasing the number of flavors leads to a decrease in the energy, as expected. In all cases, the energy is largely dominated by the N_f-body bound state as the coupling is increased. As the attractive interaction is thus enhanced by the addition of fermion species, a natural question is whether new bound states arise as N_f is increased (i.e., beyond the one at $N/N_f = 1$). We find that this is not the case; likely the appearance of new bound states requires a finite-range interaction, as is the case in 1D (see, e.g., [53]).

[1] *40 Years of Berezinskii-Kosterlitz-Thouless Theory*, edited by J. V. Jose (World Scientific, Singapore, 2013); V. L. Berezinskii, Sov. Phys. JETP **34**, 610 (1972) ; J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz, *ibid.* **7**, 1046 (1974).

[2] M. G. Ries, A. N. Wenz, G. Zürn, L. Bayha, I. Boettcher, D. Kedar, P. A. Murthy, M. Neidig, T. Lompe, and S. Jochim, Phys. Rev. Lett. **114**, 230401 (2015).

[3] P. A. Murthy, I. Boettcher, L. Bayha, M. Holzmann, D. Kedar, M. Neidig, M. G. Ries, A. N. Wenz, G. Zürn, and S. Jochim, Phys. Rev. Lett. **115**, 010401 (2015).

[4] K. Fenech, P. Dyke, T. Peppler, M. G. Lingham, S. Hoinka, H. Hu, and C. J. Vale, Phys. Rev. Lett. **116**, 045302 (2015).

[5] I. Boettcher, L. Bayha, D. Kedar, P. A. Murthy, M. Neidig, M. G. Ries, A. N. Wenz, G. Zrn, S. Jochim, and T. Enss, Phys. Rev. Lett. **116**, 045303 (2015).

[6] K. Martiyanov, V. Makhalov, and A. Turlapov, Phys. Rev. Lett. **105**, 030404 (2010).

[7] M. Feld, B. Fröhlich, E. Vogt, M. Koschorreck, and M. Köhl, Nature (London) **480**, 75 (2011).

[8] B. Fröhlich, M. Feld, E. Vogt, M. Koschorreck, W. Zwerger, and M. Köhl, Phys. Rev. Lett. **106**, 105301 (2011).

[9] S. K. Baur, B. Fröhlich, M. Feld, E. Vogt, D. Pertot, M. Koschorreck, and M. Köhl, Phys. Rev. A **85**, 061604 (2012).

[10] P. Dyke, E. D. Kuhnle, S. Whitlock, H. Hu, M. Mark, S. Hoinka, M. Lingham, P. Hannaford, and C. J. Vale, Phys. Rev. Lett. **106**, 105304 (2011).

[11] A. T. Sommer, L. W. Cheuk, M. J. H. Ku, W. S. Bakr, and M. W. Zwierlein, Phys. Rev. Lett. **108**, 045302 (2012).

[12] Y. Zhang, W. Ong, I. Arakelyan, and J. E. Thomas, Phys. Rev. Lett. **108**, 235302 (2012); M. Koschorreck, D. Pertot, E. Vogt, B. Fröhlich, M. Feld, and M. Köhl, Nature (London) **485**, 619 (2012).

[13] A. A. Orel, P. Dyke, M. Delehaye, C. J. Vale, and H. Hu, New J. Phys. **13**, 113032 (2011).

[14] E. Vogt, M. Feld, B. Fröhlich, D. Pertot, M. Koschorreck, and M. Köhl, Phys. Rev. Lett. **108**, 070404 (2012).

[15] B. Fröhlich, M. Feld, E. Vogt, M. Koschorreck, M. Köhl, C. Berthod, and T. Giamarchi, Phys. Rev. Lett. **109**, 130403 (2012).

[16] V. Makhalov, K. Martiyanov, and A. Turlapov, Phys. Rev. Lett. **112**, 045301 (2014).

[17] W. Ong, C. Cheng, I. Arakelyan, and J. E. Thomas, Phys. Rev. Lett. **114**, 110403 (2015)

[18] M. Randeria, Physics **5**, 10 (2012).

[19] P. Pieri, Physics **8**, 53 (2015).

[20] K. Miyake, Prog. Theor. Phys. **69**, 1794 (1983).

[21] M. Randeria, J.-M. Duan, and L.-Y. Shieh, Phys. Rev. Lett. **62**, 981 (1989); Phys. Rev. B **41**, 327 (1990); S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **63**, 445 (1989); M. Drechsler and W. Zwerger, Ann. Phys. (Leipzig) **504**, 15 (1992).

[22] W. Zhang, G.-D. Lin, and L.-M. Duan, Phys. Rev. A **77**, 063613 (2008).

[23] G. Bertaina and S. Giorgini, Phys. Rev. Lett. **106**, 110403 (2011).

[24] H. Shi, S. Chiesa, and S. Zhang, Phys. Rev. A **92**, 033603 (2015).

[25] X.-J. Liu, H. Hu, and P. D. Drummond, Phys. Rev. B **82**, 054524 (2010).

[26] M. Bauer, M. M. Parish, and T. Enss, Phys. Rev. Lett. **112**, 135302 (2014).

[27] V. Ngampruetikorn, J. Levinsen, and M. M. Parish, Phys. Rev. Lett. **111**, 265301 (2013).

[28] M. Barth and J. Hofmann, Phys. Rev. A **89**, 013614 (2014).

[29] C. Chafin and T. Schäfer, Phys. Rev. A **88**, 043636 (2013).

[30] S. Chiacchiera, D. Davesne, T. Enss, and M. Urban, Phys. Rev. A **88**, 053616 (2013).

[31] S. K. Baur, E. Vogt, M. Köhl, and G. M. Bruun, Phys. Rev. A **87**, 043612 (2013).

[32] T. Enss, C. Küppersbusch, and L. Fritz, Phys. Rev. A **86**, 013617 (2012).

[33] E. R. Anderson and J. E. Drut, Phys. Rev. Lett. **115**, 115301 (2015).

[34] B. C. Mulkerin, K. Fenech, P. Dyke, C. J. Vale, X.-J. Liu, and H. Hu, Phys. Rev. A **92**, 063636 (2015).

[35] C. E. Berger, E. R. Anderson, and J. E. Drut, Phys. Rev. A **91**, 053618 (2015).

[36] M. A. Cazalilla and A. M. Rey, Rep. Prog. Phys. **77**, 124401 (2014).

[37] A. N. Wenz, G. Zürn, S. Murmann, I. Brouzos, T. Lompe, and S. Jochim, Science **342**, 457 (2013).

[38] J. Levinsen and M. M. Parish, Ann. Rev. Cold Atoms Mol. **3**, 1 (2015).

[39] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in FORTRAN*, 2nd ed. (Cambridge University Press, Cambridge, England, 1992).

[40] R. L. Stratonovich, Sov. Phys. Dokl. **2**, 416 (1958); J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959).

[41] F. F. Assaad and H. G. Evertz, in *Worldline and Determinantal Quantum Monte Carlo Methods for Spins, Phonons and Electrons*, edited by H. Fehske, R. Shnieider, and A. Weise, Computational Many-Particle Physics (Springer, Berlin 2008); D. Lee, Phys. Rev. C **78**, 024001 (2008); Prog. Part. Nucl. Phys. **63**, 117 (2009); J. E. Drut and A. N. Nicholson, J. Phys. G **40**, 043101 (2013)

[42] G. H. Golub and C. H. Van Loan, *Matrix Computations*, 3rd ed. (Johns Hopkins University Press, Baltimore, 1996).

[43] T. Busch, B.-G. Englert, K. Rzążewski, and M. Wilkens, Found. Phys. **28**, 549 (1998).

[44] Dean Lee, Phys. Rev. A **73**, 063204 (2006).

[45] S. Tan, Ann. Phys. (NY) **323**, 2952 (2008); **323**, 2971 (2008); **323**, 2987 (2008); S. Zhang and A. J. Leggett, Phys. Rev. A **77**, 033614 (2008); E. Braaten and L. Platter, Phys. Rev. Lett. **100**, 205301 (2008); E. Braaten, D. Kang, and L. Platter, *ibid.* **104**, 223004 (2010); C. Langmack, M. Barth, W. Zwerger, and E. Braaten, *ibid.* **108**, 060402 (2012); J. E. Drut, T. A. Lähde, and T. Ten, *ibid.* **106**, 205302 (2011); K. Van Houcke, F. Werner, E. Kozik, N. Prokof'ev, and B. Svistunov, arXiv:1303.6245.

[46] X.-J. Liu, Phys. Rep. **524**, 37 (2013).

[47] F. Werner, Phys. Rev. A **78**, 025601 (2008).

[48] M. Valiente, N. T. Zinner, and K. Mølmer, Phys. Rev. A **84**, 063626 (2011); **86**, 043616 (2012).

[49] V. Romero-Rochin, J. Phys. B: At. Mol. Opt. Phys. **44**, 095302 (2011).

[50] E. Braaten, in *The BCS-BEC Crossover and the Unitary Fermi Gas*, edited by W. Zwerger (Springer-Verlag, Berlin, 2012).

[51] F. Werner and Y. Castin, Phys. Rev. A **86**, 013626 (2012).

[52] S. E. Gharashi, K. M. Daily, and D. Blume, Phys. Rev. A **86**, 042702 (2012).

[53] D. Mattis and S. Rudin, Phys. Rev. Lett. **52**, 755 (1984); D. Mattis, Rev. Mod. Phys. **58**, 361 (1986); S. Rudin, Phys. Rev. A **33**, 1402 (1986); K. Chadan, N. N. Khuri, A. Martin, and T. T. Wu, J. Math. Phys. **44**, 406 (2003); P. E. Kornilovitch, Europhys. Lett. **103**, 27005 (2013).