

High-order expansion around BCS theory

G. Spada,^{1,2,3,*} R. Rossi,^{4,5,†} F. Šimkovic,^{6,7} R. Garioud,^{6,7} M. Ferrero,^{6,7} K. Van Houcke,² and F. Werner^{1,‡}

¹*Laboratoire Kastler Brossel, École Normale Supérieure - Université PSL,
CNRS, Sorbonne Université, Collège de France, 75005 Paris, France*

²*Laboratoire de Physique de l'École Normale Supérieure, ENS - Université PSL,
CNRS, Sorbonne Université, Université de Paris, 75005 Paris, France*

³*INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, 38123 Trento, Italy*

⁴*Center for Computational Quantum Physics, The Flatiron Institute, New York, NY 10010, USA*

⁵*Institute of Physics, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland*

⁶*CPHT, CNRS, École Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau, France*

⁷*Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France*

(Dated: March 23, 2021)

We demonstrate that high-order diagrammatic expansion around BCS theory is a viable generic unbiased approach for strongly correlated fermions in superconducting or superfluid phases. For the 3D attractive Hubbard model in a strongly correlated regime, we observe convergence of the diagrammatic series, evaluated up to 12 loops thanks to the connected determinant diagrammatic Monte Carlo algorithm. Our study includes the polarized regime, where conventional quantum Monte Carlo methods suffer from the fermion sign problem. Upon increasing the Zeeman field, we observe the first-order superconducting-to-normal phase transition at low temperature, and a significant polarization of the superconducting phase at higher temperature.

After the discovery of superconductivity 110 years ago [1], it took nearly half a century before Bardeen, Cooper and Schrieffer provided a microscopic explanation based on an ansatz for the many-body ground-state wavefunction – a coherent state of pairs, breaking the $U(1)$ symmetry corresponding to particle number conservation [2]. Variational minimization over this ansatz leads to the well-known BCS mean-field theory which captures not only the “BCS regime” where the attractive interaction is weak, but also the “BEC regime” where the attractive interaction is strong, suggesting a smooth crossover from a fermionic superfluid with large Cooper pairs to a Bose-Einstein condensate of small composite bosons [3]. This BCS-BEC crossover scenario, confirmed experimentally in ultracold atomic gases [4–7], is relevant to neutron matter [8, 9] and to various solid-state materials [10, 11] where s -wave pairing arises between opposite-spin electrons due to phonon-mediated attraction [12–16] or between an electron and a hole due to Coulomb interaction [17–19]. The problem becomes even more interesting in presence of a Zeeman field h , *i.e.*, a chemical potential offset between $\uparrow$ and $\downarrow$ fermions, which favors a difference between $\uparrow$ and $\downarrow$ densities, and tends to destabilize the fully paired superconducting state.

The minimal theoretical formulation of the BCS-BEC crossover problem is the attractive Hubbard model on the cubic lattice, which was widely studied at $h = 0$ (and generic filling [20]) by BCS mean-field theory [21], different versions and extensions of the T-matrix approximation [11, 22, 23], dynamical mean-field theory (DMFT) in the normal [16, 24–29] and the superconducting [15, 30–35] phase, and the dynamical vertex approximation [36]. Unbiased studies, based on the auxiliary field quantum Monte Carlo (AFQMC) [37–43] or determinant diagrammatic Monte Carlo (DDMC) methods [44, 45], are mostly

restricted to a Zeeman field $h = 0$: In the $h \neq 0$ regime, where there is no symmetry between $\uparrow$ and $\downarrow$, these methods are plagued by the infamous fermion sign problem [46], and most studies resort to the static [21, 47, 48] or dynamical [49–51] mean-field approximations. A very different route is to emulate the Hubbard model with cold atoms, although long-range order in 3D was not reached so far [5, 7, 52–56].

In this Letter, we demonstrate that unbiased accurate results in the polarized superconducting phase can be obtained from a high-order diagrammatic expansion around the BCS hamiltonian. By extending the connected determinant (CDet) algorithm [57] to anomalous propagators, we go up to twelve-loop order and observe convergence of the series. This extends to superconducting phases the realm of controlled diagrammatic computations for strongly correlated fermions, which was so far limited to normal phases [58–78] with the notable exception of [79]. We determine the critical Zeeman field where a first-order superconducting-to-normal phase transition takes place at low temperature, and find a significant polarization of the superconducting phase at higher temperature. Our results deviate very substantially from the BCS mean-field predictions and provide reliable benchmarks to guide optical-lattice experiments.

The Hubbard model is defined by the hamiltonian

$$H = H_{\text{kin}} - \sum_{\sigma=\uparrow,\downarrow} \mu_{\sigma} N_{\sigma} + H_{\text{int}} \quad (1)$$

where the kinetic part is a nearest-neighbor hopping, $H_{\text{kin}} = -t \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c.$ and the interaction is on-site, $H_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow}$. Here $c_{i\sigma}$ are the fermion annihilation operators, $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ and $N_{\sigma} = \sum_i n_{i\sigma}$ the single-site and total particle-number-operators, and

$\mu_{\uparrow/\downarrow} = \mu \pm h$ the chemical potentials.

To set up a diagrammatic expansion for the infinite-size system in the superconducting phase, we must expand around an unperturbed hamiltonian H_0 that breaks the $U(1)$ symmetry. We take

$$H_0 = H_{\text{kin}} - \sum_{\sigma} \mu_{0,\sigma} N_{\sigma} + H_{\text{pair}}^{(\Delta_0)} \quad (2)$$

with a symmetry-breaking pairing term

$$H_{\text{pair}}^{(\Delta_0)} := \Delta_0 \sum_{\mathbf{i}} c_{\mathbf{i}\uparrow}^{\dagger} c_{\mathbf{i}\downarrow}^{\dagger} + h.c. \quad (3)$$

The most natural choice for the free parameters Δ_0 and $\mu_{0,\sigma}$ is given by the self-consistency conditions of BCS mean-field theory

$$\mu_{0,\sigma} = \mu_{\sigma} - U \langle n_{0,-\sigma} \rangle_{H_0} \quad (4)$$

$$\Delta_0 = -U \langle \hat{\mathcal{O}} \rangle_{H_0} \quad (5)$$

where $\langle \hat{\mathcal{O}} \rangle := \langle c_{0\uparrow} c_{0\downarrow} \rangle$ is the order parameter for the superconducting phase with long-range order in the s -wave pairing channel. In what follows we will denote this mean-field choice of Δ_0 by Δ_{MF} . We will also use other values of Δ_0 , but always keep the mean-field choice (4) for the unperturbed chemical potential.

As usual we then introduce a hamiltonian that depends on a formal parameter ξ ,

$$H_{\xi} = H_0 + \xi (H - H_0), \quad (6)$$

expand intensive observables in powers of ξ , and finally set $\xi = 1$. For the order parameter, this means introducing

$$\mathcal{O}(\xi) := \langle \hat{\mathcal{O}} \rangle_{H_{\xi}} \equiv \text{Tr}(\hat{\mathcal{O}} e^{-\beta H_{\xi}}) / \text{Tr} e^{-\beta H_{\xi}} \quad (7)$$

and expanding $\mathcal{O}(\xi) = \sum_{N=0}^{\infty} \mathcal{O}_N \xi^N$. We will see numerically that this series converges at $\xi = 1$. We can thus obtain the physical order parameter simply by evaluating the series $\sum_{N=0}^{\infty} \mathcal{O}_N$.

Thermodynamic limit and spontaneous symmetry breaking. Here it is actually crucial to work directly in the thermodynamic limit [80]. This limit should be taken in the definition (7) of $\mathcal{O}(\xi)$, and hence the thermodynamic limit should be taken before summing the $\mathcal{O}_N$ over N . Indeed, recall that in presence of spontaneous symmetry breaking, the order parameter is defined by introducing an external symmetry-breaking field η that couples to the order parameter, and sending η to zero *after* taking the thermodynamic limit:

$$\mathcal{O} = \lim_{\eta \rightarrow 0^+} \lim_{L \rightarrow \infty} \langle \hat{\mathcal{O}} \rangle_{H^{(\eta)}, L} \quad (8)$$

where $H^{(\eta)} := H + H_{\text{pair}}^{(\eta)}$ and L is the linear system size. Let us denote by $\mathcal{O}_L(\xi)$ and $\mathcal{O}_{N,L}$ the finite-system versions of $\mathcal{O}(\xi)$ and $\mathcal{O}_N$. Since there is no spontaneous

symmetry breaking for a finite system, $\mathcal{O}_L(\xi = 1) = 0$. What we should do instead, to obtain the order parameter defined in (8), is to first take the thermodynamic limit: $\mathcal{O} = \lim_{\xi \rightarrow 1} \lim_{L \rightarrow \infty} \mathcal{O}_L(\xi)$. This follows simply from (8) and the fact that H_{ξ} contains a symmetry-breaking field which by construction vanishes in the limit $\xi \rightarrow 1$ where the symmetry of the physical hamiltonian is restored. Explicitly, $H_{\xi} = H_{\text{kin}} - \sum_{\sigma} [(1-\xi) \mu_{0,\sigma} + \xi \mu_{\sigma}] N_{\sigma} + (1-\xi) H_{\text{pair}}^{(\Delta_0)} + \xi H_{\text{int}}$, which is equal to $H^{(\eta_{\text{eff}}=(1-\xi)\Delta_0)}$ plus corrections that have no effect to leading order in the limit $\xi \rightarrow 1$.

Diagrams and CDet algorithm. Each coefficient $\mathcal{O}_N$ is a sum of connected Feynman diagrams with N vertices. We compute these coefficients up to a maximal order N_{max} using the CDet algorithm generalized to the broken-symmetry phase. In addition to the normal propagator lines, diagrams contain anomalous propagator lines, where particles are destroyed at both ends, or created at both ends. These anomalous propagators are the off-diagonal elements of the 2 by 2 propagator matrix

$$\mathcal{G}_{\alpha\alpha'}(X - X') = -\langle T \Psi_{\alpha}^{\dagger}(X) \Psi_{\alpha'}(X') \rangle_{H_0} \quad (9)$$

with the Nambu spinor notation $(\Psi_0, \Psi_1) := (c_{\uparrow}, c_{\downarrow}^{\dagger})$. Here $X \equiv (\mathbf{i}, \tau)$ stands for space and imaginary-time, and T is the time-ordering operator.

Following the CDet approach, we express the diagrammatic series for the order parameter, or for the densities, as

$$\langle \Psi_{\alpha}^{\dagger}(0) \Psi_{\alpha'}(0) \rangle_{H_{\xi}} = - \sum_{N=0}^{\infty} \frac{(\xi U)^N}{N!} \int dX_1 \dots dX_N \text{cdet}(X_1, \dots, X_N) \quad (10)$$

where $\int dX := \sum_{\mathbf{i}} \int_0^{\beta} d\tau$ with β the inverse temperature, and $\text{cdet}(X_1, \dots, X_N)$ is the sum of all connected Feynman diagrams with internal vertex positions $X_1, \dots, X_N$, which is evaluated by recursively subtracting out all disconnected diagrams from the sum of all connected plus disconnected diagrams, the latter being given by the determinant of the $(2N+1)$ by $(2N+1)$ propagator matrix

$$\begin{pmatrix} 0 & \delta_{\text{sh}} & \dots & \mathcal{G}_{00}(X_{1n}) & \mathcal{G}_{01}(X_{1n}) & \mathcal{G}_{0i_0}(X_1) \\ \delta_{\text{sh}} & 0 & \dots & \mathcal{G}_{10}(X_{1n}) & \mathcal{G}_{11}(X_{1n}) & \mathcal{G}_{1\alpha}(X_1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathcal{G}_{00}(X_{n1}) & \mathcal{G}_{01}(X_{n1}) & \dots & 0 & \delta_{\text{sh}} & \mathcal{G}_{0\alpha}(X_n) \\ \mathcal{G}_{10}(X_{n1}) & \mathcal{G}_{11}(X_{n1}) & \dots & \delta_{\text{sh}} & 0 & \mathcal{G}_{1\alpha}(X_n) \\ \mathcal{G}_{\alpha'0}(-X_1) & \mathcal{G}_{\alpha'1}(-X_1) & \dots & \mathcal{G}_{\alpha'0}(-X_n) & \mathcal{G}_{\alpha'1}(-X_n) & \mathcal{G}_{\alpha'\alpha}(0) \end{pmatrix}$$

where $X_{ij} := X_i - X_j$, and $\delta_{\text{sh}} := \langle \hat{\mathcal{O}} \rangle_{H_0} + \Delta_0/U$ is the anomalous tadpole minus a counter-term. When $\Delta_0 = \Delta_{\text{MF}}$, $\delta_{\text{sh}} = 0$, reflecting the cancellation of anomalous tadpoles by Δ_0 counter-terms. The zeros on the diagonal reflect the cancellation of normal tadpoles by chemical-potential counter-terms, ensured by (4). We will also evaluate the series for the pressure, $P(\xi) = \ln \text{Tr} \exp(-\beta H_{\xi}) / (\beta L^3) = \sum_{N=0}^{\infty} P_N \xi^N$, whose

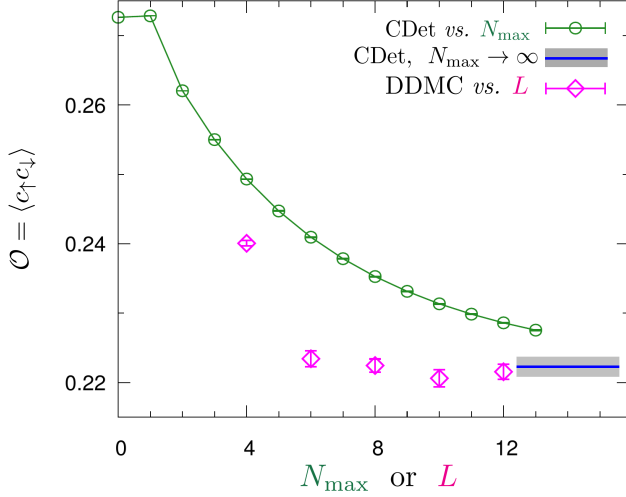


FIG. 1. *Benchmark at zero Zeeman field:* Order parameter at $T = 1/8 \approx T_c/2$. Green circles: CDet results *vs.* truncation order $N_{\max}$ ($N_{\max} = 0$ corresponds to BCS mean field theory). Blue line with grey error-band: $N_{\max} \rightarrow \infty$ extrapolated result. Pink diamonds: DDMC benchmark *vs.* system size L (CDet data are in the thermodynamic limit $L \rightarrow \infty$).

coefficients P_N are given by fully closed diagrams and are obtained with CDet by removing the last row and column from the above propagator matrix.

Our computer code is based on a library [81] providing a generic implementation of CDet, the integration over the internal vertex positions being done for all diagram orders $N \leq N_{\max}$ at once thanks to a recently introduced many-configuration Monte Carlo algorithm [82].

Results. Taking the hopping $t = 1$ as unit of energy, we set $U = -5$, and $\mu = -3.38$ so that the density $n = n_{\uparrow} + n_{\downarrow}$ is close to 0.5 particles per site, *i.e.* quarter filling – a standard choice of generic filling that differs from the special half-filled case. For $h = 0$, AFQMC is sign free and provides the critical temperature curve $T_c(U)$ [37]: Our choice of U lies in the strongly correlated regime where the curve has a broad maximum – we have $T_c(U = -5) \approx 0.25$, which is not far from the maximal value 0.33, and much larger than in the weak-coupling regime where T_c vanishes exponentially with $1/|U|$.

We start with a benchmark at $h = 0$. We compute the order parameter at $T = 1/8 \approx T_c/2$ and compare with the DDMC method [44, 83] also known as continuous-time interaction expansion in the context of impurity solvers [84–86]. Our data for the partial sum $\sum_{N=0}^{N_{\max}} \mathcal{O}_N$ converge as a function of the truncation order $N_{\max}$ to a result which agrees with the DDMC benchmark, see Fig. 1. Here and in what follows we use Padé approximants for the $N_{\max} \rightarrow \infty$ extrapolation [87]. We used $\Delta_0 = \Delta_{\text{MF}}$ and checked that the extrapolated results agree for different choices of Δ_0 .

We turn to the polarized regime $h > 0$, where conventional approaches such as AFQMC and DDMC have a

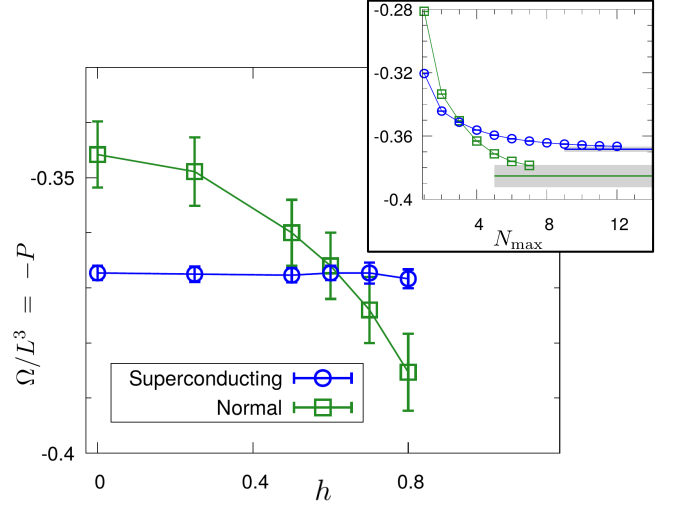


FIG. 2. *Grand-potential density vs. Zeeman field,* at $T = 1/16 \approx T_c/4$. Circles: superconducting phase, obtained by expanding around BCS mean-field theory ($\Delta_0 = \Delta_{\text{MF}}$). Squares: normal phase, obtained by expanding around the normal mean-field solution ($\Delta_0 = 0$). The crossing between the curves signals the first-order phase transition. Inset: same quantity *vs.* truncation order $N_{\max}$, at $h = 0.8$; horizontal lines with error bands are the $N_{\max} \rightarrow \infty$ extrapolated results also shown in the main panel.

sign problem and unbiased results are unavailable. We start by setting the temperature to $T \approx T_c/4$, increase the Zeeman field h , and compute the thermodynamic grand potential per unit volume, $\Omega/L^3 = -P$ with P the (electronic) pressure. We obtain the pressure of the superconducting phase using again the expansion around the broken-symmetry mean-field solution ($\Delta_0 = \Delta_{\text{MF}}$). We also evaluate the expansion around the normal mean-field solution ($\Delta_0 = 0$) which yields the normal-phase pressure. As shown in Fig. 2, the two curves cross, which indicates a first order phase transition. The error bars are dominated by the $N_{\max} \rightarrow \infty$ extrapolation, and are larger for the normal phase because we could only evaluate the series up to order 7, instead of 12 for the superconducting phase. We attribute this difference to the fact that the superconducting-phase propagators are gapped, and hence decay faster with position, which reduces the Monte Carlo variance. Within error bars, the superconducting pressure is independent of h , which means that the magnetization $m := n_{\uparrow} - n_{\downarrow}$ is zero. This indicates that we are in the regime where h is smaller than the pairing gap E_g , *i.e.* the Zeeman field is not large enough to overcome the energy cost of having an unpaired fermion, and the magnetization is exponentially suppressed at low temperature, $m \sim e^{-(E_g - h)/T}$. So the pairing gap essentially prevents the superconducting phase from polarizing, until a first-order phase transition occurs when the polarized normal phase becomes energetically favorable. Continuous-space ultracold atom experiments [88–90] and

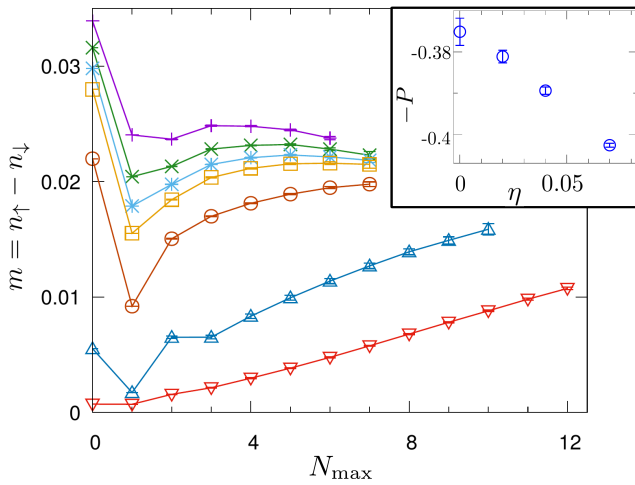


FIG. 3. Magnetization *vs.* maximal expansion order at $T = 0.19 \approx 3T_c/4$ and $h = 0.35$, for different choices of the unperturbed pairing field (from bottom to top: $\Delta_0 = 1.357 \approx \Delta_{MF}, \Delta_0 = 0.9, 0.5, 0.4, 0.37, 0.34$, and 0.3), from which we obtain $m = 0.0206(9)$. Inset: Pressure *vs.* external symmetry-breaking field η , whose slope, and hence the order parameter, is non-zero.

fixed-node Monte Carlo calculations [91] are consistent with this scenario. This is also what is predicted by BCS mean-field theory [21, 92] albeit with a critical field nearly twice larger than our unbiased result $h_c = 0.62(11)$.

For $h > h_c$ the superconducting phase is metastable. We have checked that the order parameter is still non-zero at $h = 0.8$. In this regime the convergence of the series $\sum \mathcal{O}_N$ is slower and the extrapolation becomes less stable. Therefore, instead of computing the order parameter directly, we extracted it from the response to a small symmetry-breaking field: $2\mathcal{O} = -dP^{(\eta)}/d\eta|_{\eta=0+}$, where $P^{(\eta)}$ is the pressure in presence of the field η (*i.e.* for the hamiltonian $H^{(\eta)}$), whose expansion can be extrapolated reliably [93]. As always, the notion of metastable phase has to be taken with a grain of salt: It is only well defined asymptotically close to the first-order transition point, where the energy barrier for nucleating the stable phase inside the metastable phase diverges. Accordingly, the diagrammatic expansion must actually diverge, but as long as we are not too deep in the metastable regime, this divergence is slow and only visible at very large orders, see below. Similarly, the normal phase is metastable for $h < h_c$, and we are able to follow it all the way to $h = 0$ without encountering the divergence of the series within the 7 orders that are accessible to us.

While we have seen that the pairing gap prevents the superfluid from polarizing at low temperature, the situation changes at higher temperature. At $T \approx 3T_c/4$ and $h = 0.35$, we find a magnetization $m = 0.0206(9)$, which corresponds to a polarization $(n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow)$ of 4.1%. This is 30 times larger than the BCS mean-field prediction. Therefore, BCS mean-field is not a good starting

point for the expansion in this case, and we had to tune Δ_0 away from Δ_{MF} in order to obtain convergence of the partial sums within accessible orders, see Fig. 3. Furthermore we can again check that the order parameter is non-zero by computing P *vs.* external field η , see inset of Fig. 3. We thus observe a polarized superconducting phase. This phase is possibly metastable, since its pressure (at $\eta = 0$) does not differ from the one of the normal phase within our error bars.

We end with a discussion of the large-order behavior of the expansion for the superconducting phase, which is determined by the singularities as a function of the formal expansion parameter ξ . In the limit $\xi \rightarrow 1^-$, we effectively have an external field $\eta_{\text{eff}} = (1 - \xi)\Delta_0$, hence the long-wavelength thermal fluctuations of the Goldstone mode lead to a singularity $\mathcal{O}(\xi) - \mathcal{O} \sim C\sqrt{1 - \xi}$, with $C = [\mathcal{O}/(2D_s)]^{3/2}T\sqrt{\Delta_0}/\pi$, $\mathcal{O} \equiv \mathcal{O}(\xi \rightarrow 1^-)$, and D_s the superfluid stiffness [94, 95]. This yields the power-law asymptotics $\mathcal{O}_N \sim -C/(N^{3/2}2\sqrt{\pi})$ and $P_N \sim C\Delta_0/(N^{5/2}\sqrt{\pi})$ for $N \rightarrow \infty$. When $T \rightarrow 0$ there is a crossover to the quantum-fluctuation regime where the Goldstone singularity is only logarithmic [96], leading to a faster $1/N^3$ decay of P_N . We expect another, weaker singularity at $\xi = 1$, given that the change of sign of $1 - \xi$ causes a first-order phase transition associated to a change of sign of the equilibrium order parameter. Such a first-order transition is generally expected to cause an essential singularity, with a branch-cut discontinuity $\sim e^{-B(\xi)}$ for $\xi \rightarrow 1$, with $B(\xi)$ the grand-potential barrier for nucleating a critical bubble of the stable phase inside the metastable phase [97, 98], which diverges like a power of $1/|1 - \xi|$ [99], and hence a stretched-exponential large-order behavior $\sim \exp(-\#N^a)$ with $a < 1$. In the vicinity of the physical first-order transition from Fig. 2, we expect a third singularity at a point ξ_c that moves continuously from the left to the right of the physical point $\xi = 1$ when h changes from below to above h_c , with a branch-cut discontinuity $\sim e^{-B(\xi)}$ for $\xi \rightarrow \xi_c$ with $B(\xi)$ the barrier for nucleating the stable normal phase inside the metastable superconducting phase, which diverges like a power of $1/|\xi_c - \xi|$ [100], hence a large-order behavior $(1/\xi_c)^N$ times a stretched exponential. None of these three singularities lead to a divergence of the series, except for the third one in the metastable regime where $\xi_c < 1$, but this is a slow divergence only visible at very large N as long as ξ_c is close to 1, as anticipated. In the stable regime, the Goldstone singularity dominates asymptotically, but the prefactor C is much smaller than what would correspond to our numerically obtained coefficients, assuming that D_s is not much smaller than the value 0.5 predicted by DMFT at $T = 0$ [33]. Thus at $N = 12$ we are still far from the true large- N behavior; furthermore the smallness of C implies that the contribution of the Goldstone singularity to the final result is negligible. To estimate the effect of the sub-exponential decay of the coefficients, we supplemented the Padé re-

sults with Dlog-Padé and with power-law extrapolations of the series shifted by N_s orders with $|N_s| \leq 3$, and we increased the final error bars to include all obtained results. As seen in Fig. 2 and in the inset of Fig. 3, the resulting error bars are still remarkably small. In this sense, 12 loops are sufficient for accurate extrapolation.

Outlook. BCS mean-field theory predicts [47] that in a large part of the phase diagram, the true equilibrium state is an exotic FFLO [101] phase. This open question can be tackled with the present approach by making Δ_0 space dependent. Stronger couplings can be accessed by replacing the bare interaction vertex with the T-matrix, following [102]. This would allow to look for the breached-pair gapless superconducting phase [49] and to extend the continuous-space approach of [58, 70, 103] to superfluid phases. For the repulsive Hubbard model, the d -wave superconducting phase is accessible by expanding around a momentum-dependent Δ_0 , as was done to second order in [104]. Another natural extension would be to go beyond the third-order expansion for open-shell nuclei [105].

Acknowledgements. We thank G. Biroli, E. Burovski, Y. Castin, N. Dupuis and J. Kurchan for discussions. We acknowledge support from the Paris Île-de-France region in the framework of DIM SIRTEQ (G.S.), H2020/ERC Advanced grant Critisup2 No. 743159 (F.W.), and the Simons Foundation through the Simons Collaboration on the Many Electron Problem (F.S. and M.F.). The Flatiron Institute is a division of the Simons Foundation. This work was granted access to the HPC resources of TGCC and IDRIS under the allocations A0090510609 attributed by GENCI (Grand Equipement National de Calcul Intensif).

* gabriele.spada@lkb.ens.fr

† rrossi@flatironinstitute.org

‡ werner@lkb.ens.fr

- [1] H. Kamerlingh Onnes, Leiden Comm. **124c** (1911).
- [2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **106**, 162 (1957); *ibid.* **108**, 1175 (1957).
- [3] A. J. Leggett, J. Phys. (Paris) **42**, C7 (1980); A. J. Leggett, *Diatomic Molecules and Cooper Pairs*, in: *Modern Trends in the Theory of Condensed Matter*, ed. A. Pekalski and J. A. Przystawa (Springer, 1980).
- [4] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).
- [5] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
- [6] *The BCS-BEC Crossover and the Unitary Fermi Gas*, Lect. Notes Phys. **836**, ed. W. Zwerger (Springer, Heidelberg, 2012).
- [7] I. Bloch, J. Dalibard, and S. Nascimbène, Nature Phys. **8**, 267 (2012).
- [8] S. Gandolfi, A. Gezerlis, and J. Carlson, Annu. Rev. Nucl. Part. Sci. **65**, 303 (2015).
- [9] G. C. Strinati, P. Pieri, G. Roepke, P. Schuck, and M. Urban, Phys. Rep. **738**, 1 (2018).
- [10] R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).
- [11] P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985).
- [12] M. Capone, M. Fabrizio, C. Castellani, and E. Tosatti, Rev. Mod. Phys. **81**, 943 (2009).
- [13] S. Kasahara, T. Watashige, T. Hanaguri, Y. Kohsaka, T. Yamashita, Y. Shimoyama, Y. Mizukami, R. Endo, H. Ikeda, K. Aoyama, T. Terashima, S. Uji, T. Wolf, H. von Löhneysen, T. Shibauchi, and Y. Matsuda, PNAS **111**, 16309 (2014).
- [14] T. Ohgoe and M. Imada, Phys. Rev. Lett. **119**, 197001 (2017).
- [15] Y. Murakami, P. Werner, N. Tsuji, and H. Aoki, Phys. Rev. B **88**, 125126 (2013).
- [16] J. K. Freericks and M. Jarrell, Phys. Rev. B **50**, 6939 (1994).
- [17] L. V. Keldysh and A. N. Kozlov, Zh. Eksp. Teor. Fiz. **54**, 978 (1968) [Sov. Phys. JETP **27**, 521 (1968)].
- [18] M. Combescot, R. Combescot, and F. Dubin, Rep. Prog. Phys. **80**, 066501 (2017).
- [19] J. Wang, P. Nie, X. Li, H. Zuo, B. Fauqué, Z. Zhu, and K. Behnia, PNAS **117**, 30215 (2020).
- [20] The attractive and repulsive model are related by a transformation that exchanges doping away from half-filling and polarization. In particular the attractive doped model is equivalent to the repulsive polarized model, which is also relevant to materials [106]. The half-filled attractive model, equivalent to the unpolarized repulsive model, is a special case where the broken symmetry is $SO(3)$, and will be studied elsewhere.
- [21] A. Cichy and R. Micnas, Annals of Physics **347**, 207 (2014).
- [22] J. R. Engelbrecht, H. Zhao, and A. Nazarenko, J. Chem. Phys. Sol. **63**, 223 (2002).
- [23] H. Tamaki, Y. Ohashi, and K. Miyake, Phys. Rev. A **77**, 063616 (2008).
- [24] M. Keller, W. Metzner, and U. Schollwöck, Phys. Rev. Lett. **86**, 4612 (2001).
- [25] M. Capone, C. Castellani, and M. Grilli, Phys. Rev. Lett. **88**, 126403 (2002).
- [26] A. Garg, H. R. Krishnamurthy, and M. Randeria, Phys. Rev. B **72**, 024517 (2005).
- [27] A. Toschi, P. Barone, M. Capone, and C. Castellani, New Journal of Physics **7**, 7 (2005).
- [28] R. Peters and J. Bauer, Phys. Rev. B **92**, 014511 (2015).
- [29] S. Sakai, M. Civelli, Y. Nomura, and M. Imada, Phys. Rev. B **92**, 180503 (2015).
- [30] A. Garg, H. R. Krishnamurthy, and M. Randeria, Phys. Rev. B **72**, 024517 (2005).
- [31] A. Toschi, M. Capone, and C. Castellani, Phys. Rev. B **72**, 235118 (2005).
- [32] J. Bauer and A. C. Hewson, Europhys. Lett. **85**, 27001 (2009).
- [33] J. Bauer, A. C. Hewson, and N. Dupuis, Phys. Rev. B **79**, 214518 (2009).
- [34] A. Koga and P. Werner, Phys. Rev. A **84**, 023638 (2011).
- [35] N. A. Kuleeva, E. Z. Kuchinskii, and M. V. Sadovskii, JETP **119**, 264 (2014).
- [36] L. Del Re, M. Capone, and A. Toschi, Phys. Rev. B **99**, 045137 (2019).
- [37] A. Sewer, X. Zotos, and H. Beck, Phys. Rev. B **66**, 140504 (2002).

- [38] J. Carlson, S. Gandolfi, K. E. Schmidt, and S. Zhang, Phys. Rev. A **84**, 061602(R) (2011).
- [39] J. E. Drut, T. A. Lähde, G. Wlazlowski, and P. Magierski, Phys. Rev. A **85**, 051601(R) (2012).
- [40] M. G. Endres, D. B. Kaplan, J.-W. Lee, and A. N. Nicholson, Phys. Rev. A **87**, 023615 (2013).
- [41] S. Jensen, C. N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. **124**, 090604 (2020).
- [42] S. Jensen, C. N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. **125**, 043402 (2020).
- [43] A. Richie-Halford, J. E. Drut, and A. Bulgac, Phys. Rev. Lett. **125**, 060403 (2020).
- [44] E. Burovski, N. Prokof'ev, B. Svistunov, and M. Troyer, Phys. Rev. Lett. **96**, 160402 (2006).
- [45] O. Goulko and M. Wingate, Phys. Rev. A **82**, 053621 (2010).
- [46] Unbiased QMC methods typically face an exponential scaling of computational time with the number of fermions $\mathcal{N}$, hence limiting the accessible $\mathcal{N}$ despite tremendous efforts in various fields including condensed matter, chemistry, and lattice QCD [107–110]. Often the sign problem is eliminated using an approximate ansatz for the nodal surface [8, 91, 111–116] or for the entire wavefunction [14, 113, 117], although unbiased sign-free approaches are also being developed [43, 118].
- [47] Y. L. Loh and N. Trivedi, Phys. Rev. Lett. **104**, 165302 (2010).
- [48] Y. L. Loh and N. Trivedi, *Theoretical Studies of Superconductor-Insulator Transitions*, in: *Conductor-Insulator Quantum Phase Transitions*, edited by V. Dobrosavljevic, N. Trivedi, and J. M. Valles (Oxford University Press, 2012).
- [49] T.-L. Dao, M. Ferrero, A. Georges, M. Capone, and O. Parcollet, Phys. Rev. Lett. **101**, 236405 (2008).
- [50] A. Koga and P. Werner, J. Phys. Soc. Jpn. **79**, 064401 (2010).
- [51] E. Z. Kuchinskii, N. A. Kuleeva, and M. V. Sadovskii, JETP **127**, 753 (2018).
- [52] R. A. Hart, P. M. Duarte, T.-L. Yang, X. Liu, T. Paiva, E. Khatami, R. T. Scalettar, N. Trivedi, D. A. Huse, and R. G. Hulet, Nature **519**, 211 (2015).
- [53] A. Mazurenko, C. S. Chiu, G. Ji, M. F. Parsons, M. Kanász-Nagy, R. Schmidt, F. Grusdt, E. Demler, D. Greif, and M. Greiner, Nature **545**, 462 (2017).
- [54] W. Xu, W. R. McGehee, W. N. Morong, and B. DeMarco, Nature Comm. **10**, 1588 (2019).
- [55] P. T. Brown, E. Guardado-Sanchez, B. M. Spar, E. W. Huang, T. P. Devereaux, and W. S. Bakr, Nature Phys. **16**, 26 (2020).
- [56] M. Gall, C. F. Chan, N. Wurz, and M. Köhl, Phys. Rev. Lett. **124**, 010403 (2020).
- [57] R. Rossi, Phys. Rev. Lett. **119**, 045701 (2017).
- [58] K. Van Houcke, F. Werner, E. Kozik, N. Prokof'ev, B. Svistunov, M. J. H. Ku, A. T. Sommer, L. W. Cheuk, A. Schirotzek, and M. W. Zwierlein, Nature Phys. **8**, 366 (2012).
- [59] S. A. Kulagin, N. Prokof'ev, O. A. Starykh, B. Svistunov, and C. N. Varney, Phys. Rev. Lett. **110**, 070601 (2013).
- [60] A. S. Mishchenko, N. Nagaosa, and N. Prokof'ev, Phys. Rev. Lett. **113**, 166402 (2014).
- [61] J. Gukelberger, E. Kozik, L. Pollet, N. Prokof'ev, M. Sigrist, B. Svistunov, and M. Troyer, Phys. Rev. Lett. **113**, 195301 (2014).
- [62] Y. Deng, E. Kozik, N. V. Prokof'ev, and B. V. Svistunov, Europhys. Lett. **110**, 57001 (2015).
- [63] J. P. F. LeBlanc, A. E. Antipov, F. Becca, I. W. Bulik, G. K.-L. Chan, C.-M. Chung, Y. Deng, M. Ferrero, T. M. Henderson, C. A. Jiménez-Hoyos, E. Kozik, X.-W. Liu, A. J. Millis, N. V. Prokof'ev, M. Qin, G. E. Scuseria, H. Shi, B. V. Svistunov, L. F. Tocchio, I. S. Tupitsyn, S. R. White, S. Zhang, B.-X. Zheng, Z. Zhu, and E. Gull, Phys. Rev. X **5**, 041041 (2015).
- [64] Y. Huang, K. Chen, Y. Deng, N. Prokof'ev, and B. Svistunov, Phys. Rev. Lett. **116**, 177203 (2016).
- [65] I. S. Tupitsyn, A. S. Mishchenko, N. Nagaosa, and N. Prokof'ev, Phys. Rev. B **94**, 155145 (2016).
- [66] I. S. Tupitsyn and N. V. Prokof'ev, Phys. Rev. Lett. **118**, 026403 (2017).
- [67] W. Wu, M. Ferrero, A. Georges, and E. Kozik, Phys. Rev. B **96**, 041105(R) (2017).
- [68] M. Motta, D. M. Ceperley, G. K.-L. Chan, J. A. Gomez, E. Gull, S. Guo, C. A. Jiménez-Hoyos, T. N. Lan, J. Li, F. Ma, A. J. Millis, N. V. Prokof'ev, U. Ray, G. E. Scuseria, S. Sorella, E. M. Stoudenmire, Q. Sun, I. S. Tupitsyn, S. R. White, D. Zgid, and S. Zhang, Phys. Rev. X **7**, 031059 (2017).
- [69] J. Carlström and E. J. Bergholtz, Phys. Rev. B **98**, 241102(R) (2018).
- [70] R. Rossi, T. Ohgoe, E. Kozik, N. Prokof'ev, B. Svistunov, K. Van Houcke, and F. Werner, Phys. Rev. Lett. **121**, 130406 (2018).
- [71] K. Chen and K. Haule, Nature Comm. **10**, 3725 (2019).
- [72] F. Šimkovic, J. P. F. LeBlanc, A. J. Kim, Y. Deng, N. V. Prokof'ev, B. V. Svistunov, and E. Kozik, Phys. Rev. Lett. **124**, 017003 (2020).
- [73] A. J. Kim, F. Šimkovic, and E. Kozik, Phys. Rev. Lett. **124**, 117602 (2020).
- [74] R. Rossi, F. Šimkovic, and M. Ferrero, Europhys. Lett. **132**, 11001 (2020).
- [75] C. Lenihan, A. J. Kim, F. Šimkovic IV., and E. Kozik, Phys. Rev. Lett. **126**, 105701 (2021).
- [76] T. Schäfer, N. Wentzell, F. Šimkovic, Y.-Y. He, C. Hille, M. Klett, C. J. Eckhardt, B. Arzhang, V. Harkov, F.-M. L. Régent, A. Kirsch, Y. Wang, A. J. Kim, E. Kozik, E. A. Stepanov, A. Kauch, S. Andergassen, P. Hansmann, D. Rohe, Y. M. Vilk, J. P. F. LeBlanc, S. Zhang, A. M. S. Tremblay, M. Ferrero, O. Parcollet, and A. Georges, “Tracking the footprints of spin fluctuations: A multi-method, multi-messenger study of the two-dimensional hubbard model,” arXiv:2006.10769.
- [77] A. S. Mishchenko, N. Nagaosa, and N. Prokof'ev, “Fermi blockade of the electron-phonon interaction: why strong coupling effects may not be seen in optimally doped high temperature superconductors,” arXiv:2007.09888.
- [78] A. Wietek, R. Rossi, F. Šimkovic, M. Klett, P. Hansmann, M. Ferrero, E. M. Stoudenmire, T. Schäfer, and A. Georges, “Mott insulating states with competing orders in the triangular lattice Hubbard model,” arXiv:2102.12904.
- [79] I. S. Tupitsyn and N. V. Prokof'ev, Phys. Rev. B **99**, 121113(R) (2019).
- [80] For an analogous discussion in the context of the broken-symmetry phase of ϕ^4 theory, see M. Serone, G. Spada, and G. Villadoro, JHEP **5**, 47 (2019).
- [81] R. Rossi and F. Šimkovic, *Fast Feynman Diagrammatics*, to be published.

- [82] F. Šimkovic and R. Rossi, “Many-Configuration Markov-Chain Monte Carlo,” arXiv:2102.05613.
- [83] A. Rubtsov, arXiv:cond-mat/0302228.
- [84] A. N. Rubtsov and A. I. Lichtenstein, JETP Letters **80**, 61 (2004).
- [85] A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B **72**, 035122 (2005).
- [86] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Rev. Mod. Phys. **83**, 349 (2011).
- [87] F. Šimkovic and E. Kozik, Phys. Rev. B **100**, 121102(R) (2019).
- [88] Y. Shin, C. Schunck, A. Schirotzek, and W. Ketterle, Nature **451**, 689 (2008).
- [89] S. Nascimbène, N. Navon, K. J. Jiang, F. Chevy, and C. Salomon, Nature **463**, 1057 (2010).
- [90] N. Navon, S. Nascimbène, F. Chevy, and C. Salomon, Science **328**, 729 (2010).
- [91] S. Pilati and S. Giorgini, Phys. Rev. Lett. **100**, 030401 (2008).
- [92] G. Sarma, J. Phys. Chem. Solids **24**, 1029 (1963).
- [93] In this case, the diagrammatic series is generated by $H_{\xi}^{(n)} := H_0 + \xi (H^{(n)} - H_0)$. Accordingly, δ_{sh} is then given by $\langle O \rangle_{H_0} + (\Delta_0 - \eta)/U$.
- [94] A. Z. Patashinskii and V. L. Pokrovskii, Zh. Eksp. Teor. Fiz. **64**, 1445 (1973) [Sov. Phys. JETP **37**, 4 (1973)].
- [95] E. Brézin and D. J. Wallace, Phys. Rev. B **7**, 1967 (1973).
- [96] N. Dupuis, *private communication*; N. Dupuis, Phys. Rev. E **83**, 031120 (2011).
- [97] J. Langer, Ann. Phys. **41**, 108 (1967).
- [98] N. J. Gunther, D. J. Wallace, and D. A. Nicole, J. Phys. A **13**, 1755 (1980).
- [99] Since one can go gradually from one phase to the other by slowly rotating the order parameter, the surface tension only grows with the bubble radius R as R^{d-2} in d dimensions, leading to $B(\xi) \sim 1/|1 - \xi|^{d/2-1}$.
- [100] Here the surface tension has the standard scaling R^{d-1} , hence $\mathcal{B}(\xi) \sim 1/|\xi_c - \xi|^{d-1}$.
- [101] P. Fulde and R. Ferrell, Phys. Rev. **135**, A550 (1964), A. I. Larkin and Y. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1965)].
- [102] F. Šimkovic, R. Rossi, and M. Ferrero, Phys. Rev. B **102**, 195122 (2020).
- [103] R. Rossi, T. Ohgoe, K. Van Houcke, and F. Werner, Phys. Rev. Lett. **121**, 130405 (2018).
- [104] A. Neumayr and W. Metzner, Phys. Rev. B **67**, 035112 (2003).
- [105] A. Tichai, P. Arthuis, T. Duguet, H. Hergert, V. Somà, and R. Roth, Phys. Lett. B **786**, 195 (2018).
- [106] L. Laloux, A. Georges, and W. Krauth, Phys. Rev. B **50**, 3092 (1994).
- [107] S. Muroya, A. Nakamura, C. Nonaka, and T. Takaishi, Prog. Theor. Phys. **110**, 615 (2003).
- [108] P. de Forcrand, PoS(LAT2009)010.
- [109] G. H. Booth, A. J. W. Thom, and A. Alavi, J. Chem. Phys. **131**, 054106 (2009).
- [110] T. Ma, L. Zhang, C.-C. Chang, H.-H. Hung, and R. T. Scalettar, Phys. Rev. Lett. **120**, 116601 (2018).
- [111] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
- [112] S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003).
- [113] D. Ceperley, Rev. Mineralogy and Geochemistry **71**, 129 (2010).
- [114] O. Juillet, A. Leprévost, J. Bonnard, and R. Frésard, J. Phys. A **50**, 175001 (2017).
- [115] M. Motta and S. Zhang, WIREs Comput. Mol. Sci. **8**, e1364 (2018).
- [116] M. Qin, C.-M. Chung, H. Shi, E. Vitali, C. Hubig, U. Schollwöck, S. R. White, and S. Zhang, Phys. Rev. X **10**, 031016 (2020).
- [117] T. Ohgoe, M. Hirayama, T. Misawa, K. Ido, Y. Yamaji, and M. Imada, Phys. Rev. B **101**, 045124 (2020).
- [118] C. Berger, L. Rammelmüller, A. Loheac, F. Ehmman, J. Braun, and J. Drut, Phys. Rep. **892**, 1 (2021).