High-order diagrammatic expansion around BCS theory

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We demonstrate that summation of connected diagrams to high order starting from a BCS hamiltonian 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 thermally activated polarization of the superconducting phase well described by quasiparticle theory.

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, 4]. This BCS-BEC crossover scenario, confirmed experimentally in ultracold atomic gases [5–7], is relevant to neutron matter [8, 9] and to various solid-state materials [10, 11] where s-wave pairing arises between opposite-spin electrons [12] or between an electron and a hole [13]. 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.

A 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 [14] by different versions and extensions of BCS mean-field theory [15, 16] and of the T-matrix approximation [11, 17], dynamical mean-field theory (DMFT) in the normal [18, 19] and the superconducting [20, 21] phase, and the dynamical vertex approximation [22]. Unbiased studies, based on the auxiliary field quantum Monte Carlo (AFQMC) [23–25] or determinant diagrammatic Monte Carlo (DDMC) [26, 27] methods, are mostly restricted to a Zeeman field $h = 0$: In the $h \neq 0$ regime, these methods are plagued by the infamous fermion sign problem [28] and most studies resort to the static [15, 20, 29, 30] or dynamical [31] 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 [9, 32].

In this Letter, we demonstrate that unbiased accurate results in the polarized superconducting phase can be obtained from a high-order diagrammatic expansion around a BCS hamiltonian. By extending the connected determinant (CDet) algorithm [33] to anomalous propagators, we go up to twelve-loop order and observe convergence of the series. This extends the realm of controlled diagrammatic computations for strongly correlated fermions in the thermodynamic limit [33–36] to superconducting phases. 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 for optical-lattice experiments.

The Hubbard model is defined by the hamiltonian

$$H = H_{\text{kin}} - \sum_{\sigma = \uparrow, \downarrow} \mu_\sigma \hat{N}_\sigma + H_{\text{int}}$$

with $\mu_{\uparrow, \downarrow} = \mu \pm h$ the chemical potentials, $H_{\text{kin}} = -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} c_{\mathbf{r} \sigma}^\dagger c_{\mathbf{r}' \sigma} + h.c.$ the nearest-neighbor hopping, and $H_{\text{int}} = U \sum_{\mathbf{r}} \hat{n}_{\mathbf{r} \uparrow} \hat{n}_{\mathbf{r} \downarrow}$ the on-site interaction ($c_{\mathbf{r} \sigma}$ are the fermion annihilation operators, while $\hat{n}_{\mathbf{r} \sigma} = c_{\mathbf{r} \sigma}^\dagger c_{\mathbf{r} \sigma}$...
and $\hat{N}_\sigma = \sum_\mathbf{r} \hat{n}_{\mathbf{r}\sigma}$ are the single-site and total particle-number operators.

To set up a diagrammatic expansion for the infinite-size system in the superconducting phase, where the $U(1)$ symmetry is spontaneously broken, we expand around the unperturbed quadratic hamiltonian

$$H_0 = H_{\text{kin}} - \sum_\sigma \mu_{0,\sigma} \hat{N}_\sigma + H^{(\Delta_0)}_{\text{pair}}$$

(2)

containing a symmetry-breaking pairing term

$$H^{(\Delta_0)}_{\text{pair}} := \Delta_0 \sum_\mathbf{r} \hat{c}_\mathbf{r}^{\dag} \hat{c}_{\mathbf{r}+\mathbf{L}} + h.c.$$  (3)

The most natural choice for the free parameters $\Delta_0$ and $\mu_{0,\sigma}$ is given by the self-consistency conditions of BCS mean-field theory

$$\Delta_0 = -\beta \langle \hat{O} \rangle_{H_0}$$  (4)

$$\mu_{0,\sigma} = \mu_\sigma - \Delta_0 \langle \hat{n}_{0,-\sigma} \rangle_{H_0}$$  (5)

where $\langle \hat{O} \rangle := \langle \hat{c}_0^{\dag} \hat{c}_0 \rangle$ 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 $\Delta_0$ by $\Delta_{\text{MF}}$. We will also use other values of $\Delta_0$, but always keep the mean-field choice [5] for the unperturbed chemical potential.

We then introduce a hamiltonian that depends on a formal parameter $\xi$,

$$H_\xi = H_0 + \xi (H - H_0),$$

(6)

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

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

(7)

(with $\beta \equiv 1/T$) and expanding $\mathcal{O}(\xi) = \sum_{N=0}^\infty \mathcal{O}_N \xi^N$.

In many cases, this series converges at $\xi = 1$; we can then obtain the physical order parameter simply by evaluating the series $\sum_{N=0}^\infty \mathcal{O}_N$. More generally, since $H_0$ already breaks the $U(1)$ symmetry, it is not necessary to cross a phase transition when increasing $\xi$ from 0 to 1, which would prevent one from obtaining the equilibrium values of observables at the physical point $\xi = 1$ by summing or resumming their Taylor expansions at $\xi = 0$.

Thermodynamic limit and spontaneous symmetry breaking. Here it is conceptually important to work directly in the thermodynamic limit [37]. 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 $\eta$ that couples to the order parameter, and sending $\eta$ to zero after taking the thermodynamic limit:

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

(8)

where $L$ is the linear system size and $H^{(\eta)} = H + H^{(\eta)}_{\text{pair}}$. 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: $\mathcal{O} = \lim_{\xi \to 1^-} \lim_{L \to \infty} \mathcal{O}_L(\xi)$. This follows simply from the fact that $H_\xi$ contains a symmetry-breaking field which by construction vanishes in the limit $\xi \to 1$ where the symmetry of the physical hamiltonian is restored.

Explicitly, $H_\xi = H_{\text{kin}} - \sum_\sigma (1 - \xi) \mu_{0,\sigma} + \xi \langle \hat{n}_{0,-\sigma} \rangle_{H_0} + \xi H^{(\Delta_0)}_{\text{pair}} + \xi H_{\text{int}}$, which is equal to $H^{(\eta_{\text{tot}} = (1-\xi) \Delta_0)} + \xi H_{\text{int}}$, the latter being given by the determinant of a matrix $\mathcal{O}_N$ with internal vertex positions $X_i$.

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 $G_{\sigma\sigma'}(X-X') = -(\langle \Psi_\mathbf{r}^\dag \mathbf{X}^\dag \Psi_{\mathbf{r}'\mathbf{X}'} \rangle_{H_0})$ with the Nambu spinor notation $(\Psi_\mathbf{r}, \Psi_{\mathbf{r}'} = (c_{\mathbf{r},\uparrow}, c_{\mathbf{r}',\downarrow})$. Here $X \equiv (\mathbf{r}, \mathbf{r}')$ 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 $(\hat{Q} := \hat{O})$ or for the densities $(\hat{Q} := \hat{n}_{0,\sigma})$ as $(\hat{Q})_{H_\xi} = Q_0 - \sum_{N=1}^\infty \langle \hat{n}_{0,\sigma} \rangle_{H_\xi} = Q_0 - \sum_{N=1}^\infty (\beta H_\xi) = Q_0 - \sum_{N=1}^\infty \xi H^{(\Delta_0)}_{\text{pair}} + \xi H_{\text{int}}$, which is equal to $H^{(\eta_{\text{tot}} = (1-\xi) \Delta_0)} + \xi H_{\text{int}}$, the latter being given by the determinant of a matrix $\mathcal{O}_N$ with internal vertex positions $X_1, \ldots, X_N$ and one external point at $X = (0,0)$ where the operator $\hat{Q}$ is acting. This function cdet is evaluated efficiently, in only $3^N$ operations, which is much faster than naive summation over the factorial number of connected diagrams. The trick is to recursively subtract out all disconnected diagrams from the sum of all connected plus disconnected diagrams, the latter being given by the determinant of a matrix constructed from the propagators $G_{\gamma\gamma'}(X_i-X_j)$ [38]. 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 coefficients $P_N$ are given by fully closed diagrams, and can be computed with CDet in a similar way. We use a recently introduced many-configuration Monte Carlo algorithm [39] to carry out the integration over the internal vertex positions for all diagram orders $N \leq N_{\max}$ at once.

Results. Taking the hopping $t$ 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.
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0, which yields the normal-phase 

c/2; Green circles: diagrammatic expansion around BCS mean-field theory truncated at order $N_{\text{max}}$. Blue line with grey error-band: $N_{\text{max}} \to \infty$ extrapolated result. Pink diamonds: DDMC benchmark vs. system size $L$.

$T_c(U)$ [22]: 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 $T_c$ decreases 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 [26, 40] also known as continuous-time interaction expansion in the context of impurity solvers [41]. Our data for the partial sum $\sum_{N=0}^{N_{\text{max}}} O_N$ converge as a function of the truncation order $N_{\text{max}}$ to a result which agrees with the DDMC benchmark, see Fig. 1. Here we used Padé approximants for the $N_{\text{max}} \to \infty$ extrapolation [22]. We used $\Delta_0 = \Delta_{\text{MF}}$ and checked that the extrapolated results agree for different choices of $\Delta_0$.

We turn to the polarized regime $h > 0$, where conventional approaches such as AFQMC and DDMC have a sign problem and unbiased results are unavailable. We start by setting the temperature to $T = 1/4 \approx T_c/4$, 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 $N_{\text{max}} \to \infty$ extrapolation, and are larger for the normal phase where 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 for adding an extra “unpaired” fermion, and the magnetization is exponentially suppressed at low temperature, $m \lesssim e^{-\beta (E_g - h)}$. 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. Ultracold atom experiments [43] and fixed-node Monte Carlo calculations [44] in continuous space are consistent with this scenario. This is also what is predicted by BCS mean-field theory [15, 45] albeit with a critical field nearly twice larger than our unbiased result $h_c = 0.61(12)$.

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 $\sum O_N$ 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: $\frac{\partial}{\partial \eta} P(n) \big|_{\eta = 0^+}$, where $P(n)$ is the pressure in presence of the field $\eta$ (i.e. for the Hamiltonian $H^{(n)}$), whose expansion can be extrapolated reliably. 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. 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.

We turn to higher temperature, where we can resolve the polarization of the superconducting phase, although it remains suppressed by the pairing gap. At $T = 3T_c/4$ and $h = 0.35$, we find a magnetization $m = 0.021(2)$, which corresponds to a polarization $(n_+ - n_-)/(n_+ + n_-)$ of 4%. 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 $\Delta_0$ away from $\Delta_{MF}$ in order to obtain convergence of the partial sums within accessible orders, see Fig. 3 (we used the Fastest Apparent Convergence principle to produce the final value and error bar). Furthermore we can again check that the order parameter is non-zero by computing $P$ vs. external field $\eta$, see inset of Fig. 3. We thus observe a polarized superconducting state. This state is possibly metastable, since its pressure (at $\eta = 0$) does not differ from the one of the normal phase within our error bars.

To probe the nature of this polarized superconducting state, we repeat the computation of the magnetization for different values of $h$ at fixed $T$, and fit our data with the expression $m(h, T) \approx n_{qp}(T) \sinh(\beta h)$ which holds for the usual effective low-energy theory of fermionic superfluids in terms of “unpaired fermion” quasi-particle excitations. As seen in Fig. 4, the agreement is very good, except at the largest $h$, where interactions between quasiparticles might become significant. The fit yields $m_{qp}(T) = 0.007(8)$ for the density of quasiparticles at $h = 0$, which is bounded from above by $2e^{-\beta E_g}$, hence a bound on the gap $E_g < 1.1$.

Finally, we address the large-order behavior of the expansion in the superconducting phase. We observe that $H_\xi$ contains a symmetry-breaking field that vanishes linearly for $\xi \to 1$. This implies that $O(\xi)$ contains a singularity $\propto 1/\sqrt{1-\xi}$ for $\xi \to 1$ [46]. Taylor expanding the square root gives the large-order behavior $O_N \propto 1/N^{3/2}$ and $P_N \propto 1/N^{5/2}$. Hence the coefficients do not decay exponentially, as one may have naively expected, but only like a power law. Still, the decay is sufficiently fast for the series to be convergent. To estimate the effect of the sub-exponential decay of the coefficients on our infinite-order extrapolations for the pressure, we supplemented the Padé results with Dlog-Padé and power-law extrapolations, and we increased the final error bars to include all obtained results. The resulting error bars are still remarkably small. In this sense, 12 loops are sufficient for accurate extrapolation.

In conclusion, connected diagrammatic expansions enable efficient, unbiased computations inside superconducting phases of strongly correlated fermions. Computations can be extended into metastable regimes, which allows one to locate first order transitions. Accurate results can be obtained even when they strongly differ from BCS mean-field predictions.

The applicability of the approach goes far beyond the present proof of principle. FFLO phases, which BCS
mean-field theory to predicts to be the true equilibrium state in a large part of the phase diagram [29], can be accessed by making $\Delta_0$ space dependent. Stronger couplings may be accessible by using renormalized expansions, following [36, 16]; this would allow one to look for the breached-pair gapless superconducting phase [31] and to extend the continuous-space approach of [35] to superfluid phases. For the repulsive Hubbard model, the $d$-wave superconducting phase is accessible by expanding around a momentum-dependent $\Delta_0$, as was done to second order in [41]. Another natural extension would be to go beyond third-order expansions for open-shell nuclei [50] or neutron matter [51].

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For fermions or frustrated spins, unbiased QMC methods typically face an exponential scaling of computational time with system size, which limits the accessible system sizes despite tremendous efforts in various fields including condensed matter, chemistry, and lattice QCD [54]. Often the sign problem is eliminated using an approximate ansatz for the nodal surface [8, 44, 55] or for the entire wavefunction [55]. There are also efforts to develop unbiased sign-free approaches [25, 56].

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See Supplemental Material, which includes [57], for additional details on effective low-energy theory, large-order behavior, CDet formulas, and numerical error control.

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