Renormalized perturbation theory at large expansion orders

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Abstract – We present a general formalism that allows for the computation of large-order renormalized expansions, effectively doubling the numerically attainable perturbation order of renormalized Feynman diagrams. We show that this formulation compares advantageously to the currently standard techniques due to its high efficiency, simplicity, and broad range of applicability. Our formalism permits to easily complement perturbation theory with non-perturbative information, which we illustrate by implementing expansions renormalized by the addition of a gap or the inclusion of Dynamical Mean-Field Theory. As a result, we present numerically exact results for the square-lattice hole-doped Fermi-Hubbard model in the low-temperature non-Fermi-liquid regime, relevant to study the pseudogap of cuprate superconductors, and show the momentum-dependent suppression of fermionic excitations in the antinodal region.

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Renormalization is one of the most fruitful ideas in physics. Originally discovered as a method to eliminate one-loop Feynman diagram infinities in quantum electrodynamics (QED) [1–4], it has notably led to one of the most precise comparison of theory and experiment [5]. The usefulness of renormalization beyond high-energy physics has soon been understood and it was applied to condensed matter physics [6,7] and especially to the theory of critical phenomena [8], which has led to the development of the perturbative renormalization group technique. As computing renormalized Feynman diagrams is at the core of our quantitative understanding of nature, it is of critical importance to find efficient strategies to successfully perform computations. Yet, evaluating a large number of diagram orders is an extremely challenging task even with modern computational facilities. For example, no 6-loop QED computation has been attempted to date, despite strong interest due to the availability of high-precision experiments. The main limitation in computing large-order contributions is the “factorial barrier” represented by the factorial growth of the number of Feynman diagrams with increasing diagram order. Diagrammatic Monte Carlo [9–14] was introduced with the idea that Feynman diagrams could be good sampling variables in strongly correlated electronic systems as they can be defined directly in the thermodynamic and continuum limits. While this approach dramatically simplified and automatized the computation of Feynman diagrams, and there are many recent advancements in this direction [15–20], it is still limited by the factorial barrier as it explicitly considers individual Feynman diagram topologies.

A recently introduced algorithm overcomes the factorial barrier by computing all connected and irreducible bare Feynman diagrams [21–24] at a computational cost growing exponentially with expansion order, which allows for the computation of an unprecedented number of Feynman diagram expansion orders directly in the thermodynamic limit. Similarly effective exponential algorithms overcoming the factorial barrier have also been found for the real-time evolution of quantum systems [25–28], allowing to reach the large-time limit in quantum impurity models.

Overcoming the factorial barrier has a decisive consequence on the computational complexity of the many-body problem: If the perturbative series has a non-zero radius of convergence, which is generically the case for fermions at finite temperature [29], the exponential convergence of the expansion implies that computing perturbation orders with exponential effort results in the polynomial complexity of the many-body problem, as
the resulting error scales polynomially with inverse computational time [30]. While polynomial complexity implies that bare expansions are remarkably powerful for fermionic systems on a lattice and at finite temperatures [15,23,31–33], they are nevertheless limited, in the strong-coupling regime, by the appearance of poles in the complex plane. In practice, these poles may prohibit the resummation of the series in vicinity of sharp crossovers [23]. Moreover, in the very low-temperature regime infrared divergencies are generically present [34]. Renormalization is the fundamental missing tool for accessing these regimes. It has been shown that optimized chemical potential shifts can already yield drastic improvements to the properties of evaluated series [15,35]. Furthermore, when considering systems directly in the continuous space, one is generally forced to perform renormalization in order to be able to even define the theory.

In this letter, we present a general formalism that allows for the numerical computation of renormalized perturbative expansions at large expansion orders. More precisely, we prove that it is possible to overcome the factorial barrier: We compute factorially-many renormalized Feynman diagrams in the spacetime representation at an exponential cost, resulting in overall polynomial complexity for fermionic systems at finite temperature, independently of the renormalization procedure. In what follows, we introduce the underlying theoretical concepts and show examples of large-order computations, of up to 10–14 orders, for the square-lattice Fermi-Hubbard model in nonperturbative regimes at and away from half-filling, where no other controlled techniques can be converged. This has been achieved by designing renormalization schemes that include non-perturbative information, such as approximate solutions from Dynamical Mean-Field Theory (DMFT) [36], improving the bare series in a way that extends its convergence radius and the applicability of perturbation theory. Finally, we show that the renormalized expansion can be used in the non-Fermi-liquid regime of the doped Hubbard model by computing the spectral function, which shows a strong suppression of antinodal quasiparticles.

While the technique introduced in this letter is general, for simplicity of presentation we consider the Fermi-Hubbard model on the square lattice, defined by the Hamiltonian [37]

\[ H = \sum_{k,\sigma} \epsilon_k \hat{c}_k^\dagger \hat{c}_k \sigma + U \sum_i \hat{c}_i \uparrow \hat{c}_i \downarrow \hat{c}_i \uparrow \hat{c}_i \downarrow, \tag{1} \]

where \( i \) is a lattice site, \( k \) is the lattice momentum, and \( \epsilon_k = -t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu \) is the bare dispersion relation. We consider the action representation of the Hamiltonian (1)

\[ S_{\text{bare}}[G_0, \xi] = -\langle \varphi | G_0^{-1} | \varphi \rangle + \int_X \xi(X) \langle \varphi_\uparrow \varphi_\downarrow | \varphi_\uparrow \varphi_\downarrow \rangle(X), \tag{2} \]

where \( \varphi_\sigma \) is a Grassmann field, \( X \) is the imaginary-time-lattice coordinate, and \( \xi(X) \) is a spacetime-dependent coupling constant. The physical result is obtained for a homogeneous coupling constant field \( \xi(X) = U \). The expansion in powers of \( \xi \) reproduces exactly the bare expansion in the spacetime representation. For example, the Green’s function

\[ G_{Y,Y'}[\xi] := -\frac{\int e^{-S_{\text{bare}}[G_0, \xi]} \varphi(Y) \bar{\varphi}(Y')}{\int e^{-S_{\text{bare}}[G_0, \xi]}}, \tag{3} \]

can be written as

\[ G_{Y,Y'}[\xi] = \sum_{n=0}^\infty \frac{1}{n!} \int_{1,...,n} G_{Y,Y'}(\{X_1, \ldots, X_n\}) \prod_{j=1}^n \xi(X_j), \tag{4} \]

where the functional derivative of \( G_{Y,Y'}[\xi] \) with respect to \( \xi(X_j) \), \( G_{Y,Y'}(\{X_1, \ldots, X_n\}) \), is the sum of all connected bare Feynman diagrams with \( X_1, \ldots, X_n \) as internal vertex positions, symmetrized with respect to permutations of the internal vertices, and with \( Y \) and \( Y' \) as external vertex positions. One-particle renormalization in the spacetime representation can be achieved by substituting \( G_0 \) with a functional of the interaction \( \xi \), which we denote by \( G_0[\xi] \) (see footnote 1):

\[ (G_0[\xi])^{-1} =: G_R^{-1} + \Sigma_R[\xi]. \tag{5} \]

The functional \( G_0[\xi] \) is equal to an arbitrary \( G_R \) at zero interaction, and it coincides with the physical bare propagator \( G_0 \) for \( \xi(X) = U \), at the value of the interaction strength \( U \) of interest. There are no restrictions on the functional \( \Sigma_R[\xi] \), in particular it can be defined as an infinite series in \( \xi \) without computational overhead. We can now define the renormalized action functional as

\[ S_R[G_R, \xi] := S_{\text{bare}}[G_0[\xi], \xi] \tag{6} \]

and use it to define the Green’s function as the \( \xi \) functional

\[ G_{Y,Y'}[\xi] := -\frac{\int e^{-S_R[G_R, \xi]} \varphi(Y) \bar{\varphi}(Y')}{\int e^{-S_R[G_R, \xi]}}. \tag{7} \]

The sum of all renormalized Feynman diagrams for fixed symmetrized spacetime positions is then obtained by expanding in powers of \( \xi \), \( G_{Y,Y'}(\{X_1, \ldots, X_n\}) \) from eq. (4) is the sum of all symmetrized renormalized Feynman diagrams with internal vertex positions \( X_1, \ldots, X_n \). For example, the fully renormalized one-particle scheme is obtained by imposing \( \Sigma_R[\xi] \) such that \( G(\xi) \) is a constant functional identical to \( G_R \): \( G_{Y,Y'}[\xi] = G_{R,Y,Y'} \). In this case, \( \Sigma_R[\xi] \) can be diagrammatically constructed as the sum of all two-particle irreducible diagrams. Not all renormalization schemes have a simple Feynman-diagrammatic interpretation: renormalization using Feynman diagrams becomes quickly unmanageable at large orders, as one has to keep track of all counter-terms in the general case.

\footnote{The non-functional version of this approach was introduced in ref. [38].}
A key observation is that eq. (6) implies that renormalized expansions are equivalent to bare expansions with a functional propagator $G_0[\xi]$. We introduce an efficient and general way to deal with functional expansions based on “nilpotent polynomials”, functions of $n$ commuting symbols $z_j$ such that $z_j^2 = 0$, for $j \in \{1, \ldots, n\}$. In order to compute the functional derivative of $G_{Y,Y'}[\xi]$ with respect to $\xi(X_1) \ldots \xi(X_n)$, $G_{Y,Y'}\{\{X_1, \ldots, X_n\}\}$, we only need to evaluate the functional $G_{Y,Y'}[\xi]$ for $\xi(X) = \xi_3(X) := \sum_j z_j \delta(X - X_j)$ up to linear order in each $z_j$, discarding any term of order $z_j^2$ and higher. Nilpotent polynomials of $n$ variables form a ring, where multiplication is defined as a subset convolution, which can be performed in $O(3^n)$ operations: 

\[
Q_3(z_1, \ldots, z_n) = Q_1(z_1, \ldots, z_n) \cdot Q_2(z_1, \ldots, z_n) \implies Q_3(V) = \sum_{S \subseteq V} Q_1(S)Q_2(V \setminus S), \\
\text{(8)}
\]

where $Q_1(V)$ is the coefficient of $\prod_{j \in V} z_j$. Interestingly, the recursive formula from ref. [21] which is used to compute sums of connected diagrams for the bare expansion, based on $S_{\text{bare}}[G_{0}, \xi]$, can be reinterpreted as polynomial division between two nilpotent polynomials [24]:

\[
Q_3(z_1, \ldots, z_n) = Q_1(z_1, \ldots, z_n)/Q_2(z_1, \ldots, z_n) \implies Q_3(V) = Q_1(V) - \sum_{S \subseteq V} Q_3(S)Q_2(V \setminus S), \\
\text{(9)}
\]

where $Q_2(\emptyset) = 1$ is assumed. We can therefore obtain a fast algorithm for renormalized expansions by considering a nilpotent-polynomial-valued bare propagator $G_0[\xi]$, in a similar spirit to [21]. For fermionic systems this involves computing determinants of matrices with nilpotent-polynomial entries, a task that can be performed using additions, multiplications (eq. (8)), and divisions (eq. (9)) of nilpotent polynomials.\footnote{Alternatively $O(n^{2n^2})$ operations using a fast subset convolution [39].}\footnote{For reference, we provide explicit expressions up to second perturbation order in the Supplementary Material \textit{Supplementary material.pdf}.} One can show that the computational cost to compute the sum of all symmetrized renormalized Feynman diagrams for a given configuration of interaction vertices is $O(n^{4n^2})$ (see footnote 3), much better than $(n!)^2$ which is a lower bound of the cost of enumerating all diagrams. For a series with a finite radius of convergence, this implies polynomial complexity for renormalized expansions [30].

In the regime of low temperatures and/or high interactions the bare expansion becomes very difficult to compute and evaluate, due to infrared divergencies coming from shifts of the non-interacting Fermi surface. Moreover, the presence of a superfluid instability in the attractive model \footnote{Alternatively, $O(n^{3n})$ by using fast subset convolution [39].} This comes from the fact that the computational cost is dominated by the computations of the $2^n$ determinants of nilpotent polynomials of variable order.

\[ (U < 0) \text{ reduces the radius of convergence of the series to zero at zero temperature. Two main renormalization approaches have been proposed to cure the bare expansion: The first is a fully self-consistent formalism which eliminates infrared divergencies by using the physical propagator in the expansion [14]. A known problem with this approach is that it can converge towards unphysical answers at strong interactions [40,41]. A second approach is a renormalized perturbation theory at fixed Fermi surface [34], which has the caveat of supposing the actual existence of a Fermi surface, which can be destroyed at strong interactions.}

Our goal is to construct a renormalized expansion that yields a well-behaved series, without postulating the presence of a Fermi surface. We consider the minimal renormalization scheme where the renormalized self-energy $\Sigma_R[\xi]$ is a quadratic function of the interaction $\xi$, $\Sigma_{R,X_1,X_2}[\xi] = \xi(X_1)\xi(X_2)\Sigma_{R,X_1,X_2}/U^2$ (see footnote 5). See fig. 1 for a Feynman-diagrammatic definition. Let us discuss some possibilities for $\Sigma_R$. One choice we consider is a BCS-inspired self-energy, which introduces a one-particle gap

\[ \Sigma_R = \Sigma_{\text{BCS}} = \frac{\Delta^2}{i\omega_n + \gamma \epsilon_k}, \text{ (10)} \]

where $\omega_n$ are fermionic Matsubara frequencies, and $\Delta, \gamma$ are tunable parameters. Another choice is obtained from the local DMFT self-energy

\[ \Sigma_R = \Sigma_{\text{DMFT}}^{\text{loc}}, \text{ (11)} \]

As a proof of principle we use the bare series as well as the BCS-shifted series to compute the density and double occupancy in the Hubbard atom and compare their partial sums to analytically known exact results (fig. 2). We observe perfect convergence within 10 diagram orders of the shifted series whilst the bare series strongly diverges, \footnote{We also shift the chemical potential to eliminate the mean field contribution represented by tadpole diagram $G_{0,X,X}[\xi]$ insertions, a common procedure in diagrammatic calculations.}
to the extent that it is impossible to resum. This shortcoming of the bare series is equally true for all further examples that follow.

In fig. 3, we compute the DMFT-shifted series in a strong-coupling, non-perturbative regime of the half-filled Hubbard model, where the bare series fails to converge as we are in the insulating regime. Thanks to the reduced variance after renormalization, we are able to compute 14 orders, significantly more than what is possible otherwise, and we extrapolate the result using Padé approximants [23,42,43].

In fig. 4, we show the density at small dopings and in regimes with more immediate relevance to cuprates and pseudogap physics ($t' = -0.3$, 5% doping), at low-temperatures and strong interactions. We compute the bare, BCS- and DMFT-shifted series and observe that the last mentioned series has the smallest Monte Carlo variance yielding 10–12 diagrams orders, compared to 8 orders for the first two. Both shifted series displace a negative-$U$ singularity, associated with a superfluid transition in the attractive Hubbard model [44], further away from the origin, thus simplifying the resummation procedure$^6$.

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$^6$Unlike the bare expansion results, which is physical for all $U$ (it is a simple $U$ expansion), generally the renormalized results are physical only for a chosen $U$ point. As our shift is quadratic in $U$, the renormalized expansion will be physical also for $-U$, where the system is in the superfluid s-wave phase at low temperature. This explains the oscillations as a function of the orders seen for both shifts: the system has a singularity at $-U$ for physical reasons, therefore the series cannot converge at $U$. 

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to the renormalization of the one-particle propagator for the 2D hole-doped Fermi-Hubbard model, where our formalism gave access to non-perturbative regimes at low-temperature and strong interactions, beyond the reach of current numerical techniques, enabling us to illustrate robust signatures of pseudogap physics in the spectral function. Our formalism can be straightforwardly applied to the renormalization of vertex functions, necessary to access even lower temperatures where superconductivity is expected. The paradigmatic electron gas model, where the renormalization of the Coulomb interaction is necessary to define the model in the thermodynamic limit, could be another important future application. More generally, we believe that our formalism has the potential to yield significant improvements of Feynman-diagrammatic computations in quantum chromodynamics, high-energy, solid-state, and statistical physics.

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