Feynmann’s solution of the quintessential problem in solid state physics

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Two of the most influential ideas developed by Richard Feynman are the Feynman diagram technique [1] and his variational approach [2]. The former provides a powerful tool to construct a systematic expansion for generic interacting system, while the latter allows optimization of a perturbation theory using a variational principle. Here we show that combining a variational approach with a new diagrammatic quantum Monte Carlo method [3–9], both based on the Feynman’s original ideas, results in a powerful and accurate solver to the generic solid state problem, in which a macroscopic number of electrons interact by the long range Coulomb repulsion. We apply the solver to the quintessential problem of solid state, the uniform electron gas (UEG) [10], which is at the heart of the density functional theory (DFT) success in describing real materials, yet it has not been adequately solved for over 90 years. While some wave-function properties, like the ground state energy, have been very accurately calculated by the diffusion Monte Carlo method (DMC) [11], the static and dynamic response functions, which are directly accessed by the experiment, remain poorly understood. Our method allows us to calculate the momentum-frequency resolved spin response functions for the first time, and to improve on the precision of the charge response function. The accuracy of both response functions is sufficiently high, so as to uncover previously missed fine structure in these responses. This method can be straightforwardly applied to a large number of moderately interacting electron systems in the thermodynamic limit, including realistic models of metallic and semiconducting solids.

The success of the Feynman’s diagram technique rests on two pillars, the quality of the chosen starting point, and one’s ability to compute the contributions of high-enough order, so that the sum ultimately can be extrapolated to the infinite order. We will address the former by introducing the variationally optimized starting point, as discussed below, and we will solve the latter by developing a powerful Monte Carlo method which can sum factorially large number of diagrams while massively reducing the fermionic sign problem by organizing Feynman diagrams into “sign-blessed” groups.

In the Feynman diagrammatic approach, one splits the Lagrangian of a system, \( L \), into a solvable part \( L_0 \) and the interaction \( \Delta L = L - L_0 \). The effects of the interaction is included with a power expansion in \( \Delta L \), constructed using the Feynman diagrams. Such diagrammatic series achieves the most rapid convergence when the leading term \( L_0 \) captures the emergent collective behaviour of the system, which can be very different from the non-interacting problem [12]. In the metallic state, which is of special interest in this paper, the low temperature physics is described by the emergent quasiparticles interacting with a screened Coulomb interaction. We build an effective Feynman diagrammatic approach by explicitly encoding such physics in \( L_0 \). We screen the interaction in \( L_0 \) with a screening parameter \( \lambda \), rendering the Coulomb interaction short-ranged \((V(r) \propto \exp(-r/\lambda))/r\). Correspondingly, a \( \lambda \) counter-term must be added to \( \Delta L \) to capture the non-local effects of the Coulomb interaction with high order diagrams (see the Methods section). Similarly, we introduce an electron potential \( v_k \) which properly renormalizes the electron dispersion and also fixes the Fermi surface of \( L_0 \) to the exact physical volume, which is enforced by the Luttinger’s theorem [13] (see the Methods section). In our simulations, such choice shows the most rapid and uniform convergence of the response functions for both small and large momenta.

Motivated by Feynman’s variational approach [2], we take the screening parameter \( \lambda \) as variational parameters which should be optimized to accelerate the rate of convergence. It was shown in the development of optimized perturbation theory [14] and variational perturbation theory [15] that the best choice of a variational parameter is the value at which the targeted observable is least sensitive to the change of the parameter. This technique is called the principle of minimal sensitivity (PMS). In Refs. [16–19], it was shown that the perturbative expansion optimized with the PMS can succeed even when interaction is strong, and regular perturbation theory fails. In this work, we optimize the screening parameter \( \lambda \) with PMS and observe a vast improvement to the convergence of the targeted response functions with expansion order.

While our setup of the expansion (with the static screening and the physical Fermi surface) is not entirely new [20–23], its evaluation to high enough order until ultimate convergence, has not been achieved before in any realistic model containing long-range Coulomb interaction, as relevant for realistic solids. Our solution employs a recently developed diagrammatic Monte Carlo algorithm [3–5, 8], which is here optimized to take a maximal advantage of the sign blessing in fermionic sys-
FIG. 1: The grouping of Feynman diagrams is achieved by leveraging the fermionic crossing symmetry and the free-energy generating functional. Orange top box shows the number of Feynman/Hugenholtz/Free-energy Hugenholtz diagrams at orders 3-6, excluding diagrams with the Hartree-Fock terms. The green panel on the left shows an example of the free-energy Hugenholtz diagram. The green panel on the right shows how is the Hugenholtz vertex related to the standard Feynman diagram. Note that a single Hugenholtz diagram with 

\[ \sum_{k=0}^{N} \frac{1}{k!} \frac{d^k}{dq^k} \]

represents up to \( 2^N \) standard Feynman diagrams with alternating signs. By attaching two external vertices to different propagators in the Hugenholtz free energy diagram in the green box, one generates four groups of standard Feynmann diagrams for the polarization function. Two of them are shown in the blue and orange box below. By the process of attaching external vertices to a single Hugenholtz free energy diagram, we generate 10 out of 11 standard Feynman diagrams for the polarization at the third order. The color lines represent our choice for momentum loops, which are uniquely determined by the choice of the loops in the free energy Hugenholtz diagram. Note that such grouping of diagrams allows us to calculate the weight of all diagrams in this figure with only 8 different electron propagators, instead of expected 36.

Finally, beyond variationally optimizing the zeroth order term \( L_0 \) we can also look for improvement of the high-order vertex functions. One of our choices is to sum up all ladder diagrams at the first order (see the Method and Fig.1 in the supplementary material). We will call this scheme the Vertex Corrected Constant Fermi Surface (VCCFS) scheme, and we will show in the supplementary material that it can be justified on the basis of the Baym-Kadanoff approach for conserving approximations [1]. We also use a scheme in which the ladder vertex is attached symmetrically on the left and the right side, which we call Double Vertex Corrected Constant Fermi Surface (DVCCFS) scheme. The original diagrammatic expansion, which starts with a single diagram at the first order, is here called Constant Fermi Surface (CFS) scheme. The name originates in the above described principle that electron potential \( v_{\mathbf{k}} \) is determined in such a way that \( L \) and \( L_0 \) share the same physical Fermi surface volume.
All results in this work are obtained at temperature \( T = 0.04E_F \), which is much lower than any other scale in the problem, hence results are the zero temperature equivalent. We want to point out that finite temperature calculations are very hard in the Diffusion Monte Carlo (DMC), while our method is very well suited for finite temperature calculations, and converges even faster with the increasing order. While wave-function properties, such as energy and pair distribution function, are very precisely computed by DMC, and some of them are also amenable to approximations such as GW [27, 28], the response functions are more challenging to evaluate with the existing techniques. The strength of our approach is that it can be used to compute both the static and the dynamic, the single and the multiparticle correlation functions. In Figs. 2 and 3 we show the momentum-dependent (Pauli) spin susceptibility at zero frequency, which has never been precisely calculated before to our knowledge even though its overall shape is crucial for the understanding of the quasiparticle properties [29].

The optimization of \( \chi_s(q = 0, \omega = 0) \) versus the screening parameter \( \lambda \) within (a) CFS and (b) VCCFS scheme. A single extremum at the optimized \( \lambda^* \) appears, which is however order dependent (\( \lambda^*_N \)). (c) The value of the optimized \( \chi(q = 0, \omega = 0)[\lambda^*] \) versus diagram order in both schemes. (d) The momentum dependent \( \chi(q, \omega) \) at the converged order \( N = 6 \) and optimized \( \lambda^*_N = 1.0 \) in both CFS and VCCFS schemes, and its comparison with Random phase approximation (RPA), which is exact when interaction is ignored.

FIG. 2: Spin susceptibility of UEG at \( r_s = 4 \) (i.e., density \( n = 2/(4\pi r_s^3) \)). The optimization of \( \chi_s(q = 0, \omega = 0) \) versus the screening parameter \( \lambda \) within (a) CFS and (b) VCCFS scheme. A single extremum at the optimized \( \lambda^* \) appears, which is however order dependent (\( \lambda^*_N \)). (c) The value of the optimized \( \chi(q = 0, \omega = 0)[\lambda^*] \) versus diagram order in both schemes. (d) The momentum dependent \( \chi(q, \omega) = 0 \) at the converged order \( N = 6 \) and optimized \( \lambda^*_N = 1.0 \) in both CFS and VCCFS schemes, and its comparison with Random phase approximation (RPA), which is exact when interaction is ignored.

In Figs. 3a we show the same spin-susceptibility as in Fig. 2, but for other values of density parameter \( r_s = 1 - 4 \) (here density \( n = 3/(4\pi r_s^3) \)). Finally, Fig. 3 displays the local field correction, which measures the correction of the electron correlations to the non-interacting electron gas, in which the Random phase approximation (RPA) is exact, \( G(q) \equiv \frac{q^2}{\pi^2}(\chi_{RPA}(q, \omega = 0) - \chi^{-1}(q, \omega = 0)) \). It is a very sensitive measure of correlations. It has been suggested in the literature that the possible peak near \( k \sim 2k_F \) is of great importance in the understanding of the quasiparticle properties [29].

The susceptibility also plays a central role in construction of the DFT exchange-correlation kernel. Within the local density approximation, the function \( G(q) \) is taken
to be a quadratic parabola \[^{31}\text{, which is an excellent approximation at small } q < k_F\text{, but its deviation from the quadratic function is very pronounced near } 2k_F\text{, with the hump between } k_F \text{ and } 2k_F \text{ and very steep rise at } 2k_F\].

We note that our calculation clearly shows that local field correction displays non-trivial maximum just above \(2k_F\), which is obtained for the first time to our knowledge.

**FIG. 4: Charge response and dielectric function:**

(a) The optimization of the parameter \(\lambda\) for polarization \(P(q = 0, \omega = 0)\) within CFS (when not otherwise specified) and VCCFS scheme (labeled by VC). At high orders the value is converged and constant over very extended range of values \(\lambda\). Panels (b)-(d) show the inverse of dielectric function \(1/\epsilon\) for \(r_s = 1 - 3\) at \(\lambda^*_N\), optimized for order 5, but we show \(1/\epsilon\) for all orders up to 5 and its extrapolated value. The comparison to DMC and RPA is shown. The DMC data are from Ref. \[^{30, 31}\]**. The insets of (b) and (c) show the Richardson second order extrapolation to infinite order.

For the extrapolation \(r_s\) of \(P(q = 0, \omega = 0)\) at constant \(q\) versus \(1/N\). The curve for \(N = \infty\) is obtained by the same second order Richardson extrapolation to infinite order.

Fig. 4 shows the charge response of the electron gas. Panel a displays the polarization function, defined by \(P_q = V_q^{-1}(1 - \epsilon_q)\), where \(\epsilon_q\) is the dielectric function. With the increasing diagram order, the polarization also displays a progressively optimum at \(\lambda^*\), but unfortunately both methods (CFS and LVCF) show monotonically increasing \(P_q\) with the increasing order. The inset of Fig. 2 and Fig. 3 display the convergence of \(P_q\) at \(q = 0\) with inverse order \(1/N\). For the extrapolation to the infinite order we use the standard second order Richardson extrapolation, which works well for monotonous series. Figs. 4d display the dielectric constant at \(r_s = 1\) to \(r_s = 3\) as a function of momentum \(q\) and its comparison to RPA and DMC \[^{30, 31}\]. The latter data are in agreement with our prediction, although the systematic error-bar at any finite \(q\), which are not given in the original papers but can be inferred from the fluctuations of the data points around our smooth curves, is much larger than ours, demonstrating the superiority of the newly developed VDMC method. We notice that there is a clear kink of \(1/\epsilon\) curve at \(2k_F\). This feature has been proposed in some approximations (e.g. Ref. \[^{32}\]), but the previous DMC results in Ref. \[^{30, 31}\] were not precise enough to confirm or disprove it.

\[
\begin{array}{cccccc}
 r_s & \chi_s & \chi_s/\chi^0 & P(q\omega = 0) & P^1_{DS} & P^1_{DMC} \\
 1 & 0.1093(1) & 1.122(2) & 0.1175(6) & 0.1174 & 0.1175 \\
 2 & 0.0506(2) & 1.226(5) & 0.0753 & 0.0753 & 0.0753 \\
 3 & 0.0427(3) & 1.32(1) & 0.0724 & 0.0714 & 0.0711 \\
 4 & 0.0340(4) & 1.40(2) & & & \\
\end{array}
\]

**TABLE I: Long wavelength values of spin and charge response:** First column \(\chi_s = \chi_s(q = 0, \omega = 0)\) is the spin susceptibility bracketed from below and above as shown in Fig. 4. Here \(\chi^0 = \chi_{RPA}\). \(P(q\omega = 0)\) is the long wavelength polarization as obtained by the same method. Unfortunately both CFS and VCCFS methods approach the converged value from below, hence extrapolation to \(N = \infty\) is needed, which leads to much larger error-bar in our calculation. For comparison, we show in the forth and the fifth column the corresponding DMC results, extracted from the correlation energy ansatz proposed in Ref. \[^{33}\] and Ref. \[^{34}\] respectively.

Finally, in Table I we give our best estimates for the static spin and charge response with estimation of the error-bar. Contrary to the finite momentum response, the static charge response \(P(q = 0, \omega = 0)\) can be obtained from the ground state energy of the system, and hence it can be extracted very precisely from the existing DMC calculations. We compare it with our results, and find excellent agreement. Our method allows us to compute the spin response even more precisely than the charge response because CFS and VCCFS schemes approach the exact result from below and above, hence no extrapolation is needed. These values have not been previously computed with a controlled method, and might be useful to develop better DFT functionals for magnetic materials.

The prospects of combining the variational diagrammatic Monte Carlo with DFT to obtain theoretically controlled results in real solids are particularly exciting, as the DFT potential is semi-local and can be added to \(v_k\), so that it will play a role of a counter-term in the expansion. The complexity would be modest, because no expensive self-consistency is required, and because the interaction is statically screened even at the lowest order, hence the scaling of this method should be similar to the complexity of screened hybrids \[^{35}\] rather than self-consistent GW approximation \[^{36}\].

**Method**

Using the standard Hubbard-Stratonovich transformation, the Lagrangian of the uniform electron gas can be cast into the form in which the Coulomb interaction is mediated by an auxiliary bosonic field \(\phi_Q\). Motivated by the well known fact that the long-range Coulomb interaction is screened in the solid, and that the effective potential of emerging quasiparticles differs from the bare potential, we introduce the screening parameter \(\lambda\) and an
electron potential $v_k$ into $L_0$, which then takes the form

$$L_0 = \sum_{k\sigma} \bar{\psi}_k^\dagger (\frac{\partial}{\partial \tau} - \mu + \frac{k^2}{2m} + v_k(\xi = 1)) \bar{\psi}_{k\sigma}$$

and represents well the low-energy degrees of freedom in the problem when parameters $\lambda$ and $v_k$ are properly optimized. To compensate for this choice of $L_0$, we have to add the following interaction

$$\Delta L = \sum_{k\sigma} \bar{\psi}_k^\dagger v_k(\xi) \bar{\psi}_{k\sigma} - \frac{\xi^2}{2V} \sum_{q\neq 0} \phi_q^\dagger \frac{\lambda_q}{8\pi} \phi_q$$

so that, when the number $\xi$ is set to unity, $L = L_0 + \Delta L(\xi)$ is exactly the UEG Lagrangian. The density $\rho$ is $\rho_q = \sum_{k\sigma} \bar{\psi}_k^\dagger \bar{\psi}_{k+q\sigma}$. Note that the first two terms in $\Delta L$ are the counterterms which exactly cancel the two terms we added to $L_0$ above. We use the number $\xi$ to track the order of the Feynman diagrams, so that order $N$ contribution sums all diagrams carrying the factor $\xi^N$. We set $\xi = 1$ at the end of the calculation. Note also that this arrangement bears similarity with the well established methods, such as G0W0 [36], which computes the self-energy at the lowest order ($\xi^1$) and sets $v_k$ to the DFT Kohn-Sham potential, and $\lambda_q$ to the bubble diagram ($\lambda_q = g^0 g^0$ with $g^0 = (i\omega - \mu - \frac{k^2}{2m} - v_k)$). The so-called skeleton Feynman diagram technique is recovered when $v_k$ and $\lambda_q$ are equated with the self-consistently determined self-energy and polarization. However, note that such diagram expansion can be dangerous, as it can lead to false convergence to the wrong solution [37].

In optimizing the screening parameter $\lambda_q$ by the principle of minimal sensitivity, we found it is sufficient to take a constant $\lambda_q = \lambda$. Furthermore, we found that the uniform convergence for all momenta is best achieved when the electron potential $v_k$ preserves the Fermi surface volume of $\int d\Gamma_k = \frac{\xi}{2} g^{0\dagger} + g^{0}\lambda_q^\dagger + \frac{\xi^2}{2} s_2^f + \xi^3 s_3^f \ldots$, and we determine $s_N$ so that all contributions at order $N$ do not alter the physical volume of the Fermi surface. Since the exchange ($\Sigma_{\xi}^f$) is static, and is typically large, we accomodate it at the first order into the effective potential, so that at the first order we recover the screened Hartree-Fock approximation, i.e., interaction screened to $\exp(-r\sqrt{\lambda})/r$ and optimized $\lambda$.

The vertex corrected (VC) constant Fermi surface scheme (CFS) is a conserving approximation which is derived from the Baym-Kadanoff approach by regarding the potential $v_k$ as a functional of the green’s function, i.e., $v_k(\xi^0)$, while CFS is the conserving approximation when $v_k$ is taken as a constant in the Baym-Kadanoff derivation (see the Supplementary Material). In practice, within the VCCFS scheme, we precompute the three-point ladder vertex, and attach it to each Feynman diagram on the right-hand side, and at the same time, we eliminate all ladder-type diagrams from the sampling, to avoid double-counting of diagrams. Similarly, the ladder vertex is attached on both sides in the Double Vertex Corrected Constant Fermi Surface (DVCCFS) scheme, and a few additional ladder-type diagrams are then eliminated from sampling.

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Supplementary Material

A. Conserving Diagrammatic Expansion

This section introduces two conserving diagrammatic techniques, which are called CFS and VCCFS in the main text, to calculate the polarization $P$ (or susceptibility $\chi$). Both schemes keep the exact crossing symmetry and conservation laws (particle number, momentum, energy, etc.) order by order. We note that the particle-number conservation law of the polarization $P(\mathbf{q} \to 0, \tau) \to const$ is essential for the Coulomb electron gas, in order to properly describe the plasmon physics.

The conserving diagrammatic expansions for the polarization can be constructed with the Baym-Kadanoff approach [1, 2], which is briefly reviewed below, before presenting the computational schemes used in the main text. In the Baym-Kadanoff approach one first introduces an external potential coupled to the density operator of the system,

$$S[\psi^+, \psi; U] = S[\psi^+, \psi] - \int d1d2 \psi^+ (1) U (1, 2) \psi(2),$$

where $\psi$ are a Grassmann field for the electrons; the indexes represent spatial, temporal and spin variables. The generating functional for the connected correlation functions is defined as $\ln Z[U]$ with,

$$Z[U] = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^+, \psi; U]}.$$  

For a given approximation to $\ln Z[U]$, one can derive a conserving approximation for the one-particle Green’s function by making sure that

$$G(1, 1') = \frac{\delta \ln Z[U]}{\delta U(1', 1)} \bigg|_{U \to 0},$$

while the two particle correlation function (charge, or spin correlation function if spin indexes are not summed), should satisfy

$$\chi(1, 2) = \frac{\delta G(2, 2^+; U)}{\delta U(1^+, 1)} \bigg|_{U \to 0},$$

where the notation $1^+$ and $2^+$ indicates the time ordering of the field operators. The polarization, for which we
will develop a diagrammatic expansion, is related to the correlation function $\chi$ by

$$\chi(1, 2) = -P(1, 2) + \int d3d3' P(1, 3) v_{\text{bare}}(3, 3') \chi(3', 2),$$

where $v_{\text{bare}}$ is the unscreened Coulomb interaction. Note that the second term vanishes for the spin correlation function $\chi_{zz}$ in the unpolarized electron gas.

We will apply the above algorithm to the uniform electron gas model defined by the Lagrangian $L = L_0 + \Delta L$, where the solvable part is

$$L_0 = \sum_{k\sigma} \psi_{k\sigma}^\dagger \left( \frac{\partial}{\partial \tau} - \mu + \frac{k^2}{2m} + v_k(\xi = 1) \right) \psi_{k\sigma}$$

and the correction is

$$\Delta L = - \sum_{k\sigma} \psi_{k\sigma}^\dagger v_k(\xi) \psi_{k\sigma} - \frac{\epsilon^2}{2V} \sum_{q \neq 0} \phi_q^\dagger \phi_q \lambda_q$$

This Lagrangian was introduced in the main part of the text. Here the density $\rho$ is $\rho_q = \sum_{k\sigma} \psi_{k\sigma}^\dagger \psi_{k+q\sigma}$. Note that the effective potential $v_k$ and the inverse screening length $\lambda$ in $L_0$ are compensated by the counter-terms in the correction $\Delta L$. The parameter $\xi$ is set to unity at the end of the calculation.

In the Baym-Kadanoff approach the external potential term $U(1, 2)$ should be added to the solvable part $L_0$, and then the perturbative expansion for the generating functional $\ln Z[U]$ should be carried out using the standard Feynman diagrammatic expansion with building blocks shown in Fig. 5. Note that the diagrammatic series constructed in this way only implicitly depends on the external potential $U$ through the bare electron propagator $g[U]^{-1} = -\frac{\partial}{\partial \tau} + \frac{k^2}{2m} - v_k + U$. The density $\rho$ is $\rho_q = \sum_{k\sigma} \psi_{k\sigma}^\dagger \psi_{k+q\sigma}$. Note that the interaction line 8 is proportional to $v_k(\xi)$ (the single-particle counter term) and $\xi \lambda_0$ (the interaction counter term), and are depicted in the last two diagrams.

Now we are ready to discuss the Feynman diagrammatic expansion used in our work. We will first discuss the CFS scheme. To do this, we generate all free energy diagrams of order $N-1$, for example the diagram in Fig. 1 of the main text, where the effective potential $v_k$ is regarded as an arbitrary function, independent of $U$. We then calculate the two-particle correlation function with the second derivatives with respect to external potential $U$,

$$\chi(1, 2) = \left[ \frac{\delta^2 \ln Z[U]}{\delta U(1^+, 1) \delta U(2^+, 2)} \right]_{v_k = \Sigma_1^\infty, U = 0},$$

Note that the $U$ derivative is taken by the chain rule, i.e., $\delta / \delta U = (\delta q / \delta U)(\delta / \delta q)$, where the $U$-derivative of the propagator is simple: it just splits the propagator into two by inserting an external vertex,

$$\frac{\delta q(1, 2; U)}{\delta U(3^+, 3)} = -g(1, 3)g(3, 2).$$

This relation is derived by taking the derivative of the identity $q^{-1}g = 1$, which is $gg^{-1}dg/dU + (dg^{-1}/dU)g = 0$, therefore $dg/dU = -g(dg^{-1}/dU)g$ and $dg^{-1}/dU = 1$, provided $v_k$ is independent of $U$. Diagrammatically, a derivative $\delta \Sigma$ removes a single-particle propagator from the Feynman diagram ($\delta \Sigma g$), and we then replace it with an external vertex and the two propagators, i.e., $\delta \Sigma g = -gg$. In other words, it inserts an external vertex on an existing bare electron propagator. Note that this operation increases the diagram order by one. Finally, after the derivative is taken, we substitute $v_k$ with its expression in terms of the exchange self-energy,

$$v_k = \xi (\Sigma^x_k - \Sigma^x_{k+\sigma}) + \xi^2 s_2 + \xi^3 s_3 + \cdots.$$

With the above described algorithm, we obtain the conserving expansion for the two particle correlation function $\chi$, however, the convergence for the dielectric function is even faster when the expansion is carried out for the polarization function defined by Eq. [7]. In the momentum and frequency space, the two are related by

$$\chi(q) = -\frac{P_q}{1 - P_q \frac{8\pi}{q^2 + \lambda}},$$

or $\chi(q) = -[P_q + \frac{8\pi}{q^2 + \lambda} P_q + \frac{8\pi}{q^2 + \lambda} P_q + \cdots]$, meaning that $P_q$ is the irreducible part of $\chi(q)$ with respect to cutting the interaction propagator $\frac{8\pi}{q^2 + \lambda}$. Similarly, when working with the screened interaction $\frac{8\pi}{q^2 + \lambda}$, we can rewrite

$$\frac{8\pi}{q^2 + \lambda} = \frac{8\pi}{q^2 + \lambda} \sum_{n=0}^\infty \left( \frac{8\pi}{q^2 + \lambda} \right)^n$$

and therefore

$$\chi(q) = -\frac{P_q}{1 - P_q \frac{8\pi}{q^2 + \lambda} \sum_{n=0}^\infty \left( \frac{8\pi}{q^2 + \lambda} \right)^n},$$

which shows that $P_q$ is now the irreducible part of $\chi(q)$ with respect to cutting the interaction propagator $\frac{8\pi}{q^2 + \lambda}$.
The perturbative expansion for the polarization is formulated with the standard Feynman diagrams with counterterms. The shaded block represents all one-interaction-irreducible diagrams for the particle-hole four-point vertex function. Note that the single-particle counterterm first appears at the second order, while the interaction counter-term first appears at the third order.

To derive the vertex corrected VCCFS scheme, we carry out slightly different order of operations, namely

\[
\chi(1, 2) = \frac{\delta}{\delta U(1^+, 1)} \left[ \frac{\delta \ln Z[U]}{\delta U(2^+, 2)} \right]_{V_k = \Sigma_k^q + \cdots, U=0}
\]

which means that we substitute the expression for the effective potential after the first derivative is taken (i.e., into the expression for the bare electron propagator). When taking the second derivative, we need to keep in mind that the effective potential \(v_k = v_k[U]\) now depends on \(U\) through the exchange self-energy, which is a functional of the bare propagator \(g[U]\). The chain rule is therefore modified to

\[
\frac{\delta}{\delta U} = \frac{\delta g}{\delta U} \left( \frac{\partial}{\partial g} \right)_{v_k} + \frac{\delta v_k}{\delta U} \left( \frac{\partial}{\partial v_k} \right) g.
\]

where the second derivative acts only on the single-particle counter-terms. Taking the derivative with respect to \(U\) as above gives \(d\tilde{g}/dU = -g(dg^{-1}/dU)g = -g(1 - d\Sigma^2/dU)g\), and since \(d\Sigma^2/dU = \frac{-[8\pi/(q^2 + \lambda)] \, dg/dU, \) we now need to insert a ladder vertex between the two \(g\)'s in the following way \[1\],

\[
\frac{\delta g(1, 2; U)}{\delta U(3^+, 3)} = -\int dVdV' \, g(1, 1')\Gamma_3(1', 2'; 3)g(2', 2),
\]

where the ladder vertex correction \(\Gamma_3\) is defined with a self-consistent equation as shown in Fig. 7. Similarly we can see that \(\delta v_k/\delta U = \delta\Sigma^2/\delta U = \delta g/\delta U\), where \(\delta g/\delta U\) is given by Eq. 15.

This operation then gives the diagrammatic expansion for the two-particle correlation function, similar to the previous CFS scheme, except that the external vertex on one side has to be replaced by the ladder vertex corrections \(\Gamma_3\), and the ladder diagrams in the bare expansion on the same side are removed by the diagrams generated by the operator \(\frac{\delta^2}{\delta U \delta v_k}\). The resulting diagrams for the polarization function are again the irreducible part of \(\chi\), and are depicted in Fig. 8. Note that VCCFS scheme resumes an infinite series of ladder diagrams, and hence encodes nonperturbative effects of the charge renormalization.

We emphasize here that all polarization diagrams in both schemes only involve the statically screened Coulomb interaction \(\frac{8\pi}{q^2 + \lambda}e^2\). This is a nontrivial result, given that the definition of the polarization in Eq. (7) explicitly depends on the bare Coulomb interaction. Combining this feature with the fact that screened Coulomb interaction does not diverge in the long-wave-length limit, all polarization diagrams are now automatically regularized, making the Monte Carlo simulations much more efficient.

To improve the Monte Carlo simulations much more efficiently, we propose a systematic algorithm to organize diagrams so that an efficient diagrammatic Monte Carlo method can be implemented. To calculate the diagrams of the order \(N\), the diagramatic Monte Carlo algorithm needs to integrate over all internal variables, such as momenta and times, and also sum over all

B. “Sign-blessed” Diagram Group

In this section, we propose a systematic algorithm to organize diagrams so that an efficient diagrammatic Monte Carlo method can be implemented. To calculate the diagrams of the order \(N\), the diagramatic Monte Carlo algorithm needs to integrate over all internal variables, such as momenta and times, and also sum over all.
topologies of the diagrams, i.e.,
\[
\sum_{\text{topology}} \int [d\tau]^{2N}[dk]^{N+1} W[(\tau),\{k\}] \tag{16}
\]

Due to the Fermi statistics, the sign of the integrand $W[(\tau),\{k\}]$ alternates as the topology and internal variables change. A straightforward Monte Carlo method, which samples the absolute value of the integrand $|W[(\tau),\{k\}]|$, suffers from the notorious sign problem. In this work, we overcome this problem by organizing the sign-alternating diagrams into the “sign-blessed” groups, and design a Monte Carlo algorithm which samples the weight of a group rather than an individual diagram. The “sign-blessed” group of diagrams is a sum of similar diagrams that largely cancel, and we denote its weight by $W_{\text{group}}[(\tau),\{k\}] = \sum_{\text{topology} \in \text{group}} W[(\tau),\{k\}]$, which is much smaller than the typical weight $W[(\tau),\{k\}]$ of an individual diagram. For a given group, the Monte Carlo integration over momenta and time,
\[
\int [d\tau]^{2N}[dk]^{N+1} W_{\text{group}}[(\tau),\{k\}] \tag{17}
\]
is then much more efficient than the algorithms which samples diagrams one by one.

The “sign-blessed” group may be obtained by grouping: i) diagrams that share the same set of internal variables, and those diagrams in which ii) the integrand $W[(\tau),\{k\}]$ massively compensate with each other. The first requirement is automatically satisfied for the connected diagrams of the same order $N$, as all order-$N$ connected diagram requires $N + 1$ independent momentum/frequency variables or $2N$ space/time variables. The second requirement is much more challenging and can only be achieved by carefully examining the sign structure of the diagrams.

We identify two useful generic rules for the occurrence of the sign-blessing in fermionic systems with momentum-imaginary-time representation. One generic mechanism which is particularly important for fermions is the crossing symmetry as depicted in Fig. 9, namely permuting arbitrary two fermionic propagators causes an overall sign change of the diagram. If two fermionic propagators being exchanged carry similar momentum, which occurs near the Fermi surface, the direct and exchange diagrams strongly compensate with each other. It is therefore important to optimally arrange the internal variables so that the diagram integrand $W_{\text{group}}$ keeps the exact crossing symmetry.

Another generic mechanism is the conservation laws (or Ward identities). For example, the conserving diagrammatic expansions for the polarization proposed in the previous section satisfy $P(q \to 0, \tau) \to 0$ when approaches the zero temperature. However, this is an emergent property satisfied only by the sum of a conserving group of diagrams. In fact, all individual polarization diagrams (except the bubble diagram) break the conservation law and fluctuate around zero. Therefore, we observe a strong sign cancellation between the diagrams in the same conserving group. According to the Baym-Kadanoff approach in Eq. (8), there is one-to-one correspondence between the minimal conserving groups for the polarization diagrams of the order $N$ and the ln $Z$ diagrams of the order $N - 1$.

Indeed, for an arbitrary ln $Z$ diagram, one can simply attach two external vertices to two of the bare electron propagators $g$ in all possible ways, and generate a conserving group for the polarization function. Strictly speaking, the sign blessing of the conserving groups is only guaranteed after integrating out all interval variables. However, provided that the internal variables of the polarization diagrams are inherited from the same free energy diagram, the operation of inserting two external vertices generates different time-ordered polarization diagrams, and leads to sign alternation within the conserving groups, implicitly encoding the sign blessing of the conservation law.

Now we are ready to propose the algorithm to group the diagrams and properly arrange interval variables. The algorithm is applicable to an arbitrary combination of momentum/frequency or space/time variables. To be consistent with the main text, we describe the algorithm with momentum/time representation. The main steps of the algorithm are:

i) Pick an arbitrary order-$N$ connected ln $Z$ diagram, label all $2N$ time variables and choose $N + 1$ independent momentum loops. Keep momentum loops as short as possible.

ii) Generate a new connected ln $Z$ diagram by permuting two electron propagators, rearrange the momentum loops as described in Fig. 9 so that they automatically form a complete and independent loop basis for the new diagram. Thanks to the crossing symmetry, the new dia-
gram has the opposite sign to the starting diagram. This step is repeated until all ln Z diagrams are exhausted.

iii) For each ln Z diagram, attach two external vertices to two of the electron propagators in all possible ways, to generate a conserving group of polarization diagrams. The arrangement of the interval variables of the original ln Z should not be modified in this step, so that the generated polarization diagrams share common parts of the diagram (many equal propagators).

It is also possible to apply the above algorithm to Hugenholtz diagrams, which form a particular subset generated by the algorithm in Eq. (9) (when the top and the bottom bosonic propagators are connected to each other). These diagrams combine the direct and exchange interaction into an antisymmetric four-point vertex. They are particularly convenient if one works with momentum/frequency, or momentum/time representation, and the interaction is instantaneous, as in our model Eq. (8) and Eq. (9).

[1] Baym, G. and Kadanoff, L. P. Conservation Laws and Correlation Functions. Phys. Rev. 124, 287-299 (1961).

[2] Baym, G. Self-Consistent Approximations in Many-Body Systems. Phys. Rev. 127, 1391-1401 (1962).

[3] To make the statement rigorous, all ln Z diagrams containing Hatree terms should be excluded from this correspondence since the polarization diagrams are one-interaction-irreducible.