

Exchange-correlation effect in the charge response of a warm dense electron gas

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The study of warm dense matter, widely existing in nature and laboratories, is challenging due to the interplay of quantum and classical fluctuations. We develop a variational diagrammatic Monte Carlo method and determine the exchange-correlation kernel $K_{XC}(q; T)$ of a warm dense electron gas for a broad range of temperature T and momentum q . We observe several interesting physics, including the T -dependent evolution of the hump structure and the large- q tail and the emergence of a scaling relation. Particularly, by deriving an analytical form for $q \rightarrow \infty$, we obtain large- q tails of K_{XC} with high precision. It is shown that the K_{XC} data can be reliably transformed into real space, which can be directly used in density-functional-theory calculations of real warm dense matter.

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Introduction. Over the past two decades, extensive research interests have been devoted to an extreme state of matter at high temperature and density, called warm dense matter (WDM). The WDM region occurs in various astrophysical objects such as giant planet interiors [1–5], brown dwarfs [6,7], and neutron crusts [8]. Nowadays, it can be routinely realized and probed in novel high-power laser and accelerator facilities [9–12]. The electrons in WDM are about to lose quantum coherence while still demonstrating nontrivial quantum corrections, resulting in a special crossover state between classical plasma and quantum condensed matter.

Within the local-density approximation treatment, the electrons in WDM are modeled by the warm dense uniform electron gas (UEG). The UEG only has two parameters, the density parameter (Wigner-Seitz radius) $r_s = \bar{r}/a_B$ and the reduced temperature $\theta = T/T_F$, where $\bar{r}$ is the average interparticle distance, a_B is Bohr radius, and T_F is the Fermi temperature. At the high-density limit ($r_s \rightarrow 0$), the electrons behave as an ideal Fermi gas; at low density, the Coulomb potential becomes dominant, eventually resulting in a Wigner crystal [13–15]. Dimensional temperature ratio θ can be seen as a quantum degeneracy parameter. In the high-temperature ($\theta \gg 1$) and zero-temperature ($\theta \rightarrow 0$) limits, the UEG has been well described by the classical plasma theory and the quantum condensed matter theory, respectively. However, due to the complicated interplay of electronic correlations, quantum coherence, and thermal fluctuations, the crossover regime $r_s \sim \theta \sim 1$, particularly relevant for WDM, is much less understood.

The density (or charge) response function, one of the most important electronic probes, is measured in many vital diagnostic experiments of WDM [16–21]. The random phase approximation (RPA) well describes the long-range screening effects and is a reasonable approximation in the weakly interacting regimes. However, it becomes invalid in the WDM conditions because the RPA response function only accounts for the Hartree component of the induced potentials [22] and overestimates the short-range correlations between electrons. The neglected exchange-correlation (XC) component can be parametrized by the local field correction (LFC),

$$G(q, \omega) = 1 - \frac{1}{v_q} \left[\frac{1}{\chi_0(q, \omega)} - \frac{1}{\chi(q, \omega)} \right], \quad (1)$$

where $\chi_0(q, \omega)$ and $\chi(q, \omega)$ are the dynamic density response functions of noninteracting and interacting systems, respectively, and $v_q = 8\pi/q^2$ is the long-range Coulomb repulsion (Rydberg atomic units are used). The LFC encodes the structure of effective electron-electron interaction and is crucial for the understanding of many experimental phenomena, exemplified by plasmon [11,23], Coulomb and spin-Coulomb drag effects [24,25], electrical and thermal conductivities [26,27], stopping power [28,29], and energy transfer rates [30]. In the time-dependent density functional theory (TDDFT) [22,31,32], the so-called XC kernel, $K_{XC}(q, \omega) = -v_q G(q, \omega)$, is typically used as an input for *ab initio* calculations of ground-state energies and electronic spectra in real materials. For small and large q , since $G(q) \propto q^2$, the behavior of G is better described by K_{XC} .

Substantial efforts have been devoted to studying the LFC of UEG, particularly its static one $G(q) \equiv G(q, \omega = 0)$. At $T = 0$, in the ground state, analytic properties of the LFC

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in the small- and large- q limits were derived [33–36] and numerical calculations of $G(q)$ were performed for various density parameters by diffusion quantum Monte Carlo [37,38]. Recently, Chen and Haule developed a variational diagrammatic Monte Carlo (VDMC) method [39] using renormalized Feynman diagrammatic expansion and used it to obtain accurate results on the static density LFC [39] and spin LFC [40] for $r_s \leq 5$. Furthermore, the dynamic LFC was computed by implementing the algorithmic Matsubara integration with the VDMC [41]. For finite T , calculations of $G(q)$ are amenable due to the recent development of unbiased path-integral Monte Carlo (PIMC) methods [42–45]. Dornheim *et al.* [46] reported a neural-network representation of $G(q)$ based on PIMC data and ground-state parametrization [47]. They further gave an analytic parametrization of $G(q)$ within effective static approximation [48] and used it to describe the response functions in the WDM regime [49,50].

Many challenges still exist. First, due to the limited precision of ground-state data, it remains controversial whether the LFC develops a peak structure near $q = 2k_F$ (where k_F is the Fermi momentum), termed the “ $2k_F$ hump puzzle” [51]. Second, the PIMC methods suffer from the notorious sign problem [52–54] as the electrons become a degenerate quantum liquid for $T < T_F$ [55]. Therefore, our current knowledge has a significant gap: how the LFC evolves from zero T in the ground state, via low T relevant for condensed matter physics and intermediate T corresponding to WDM, and finally to high T relevant for classical plasma. Third, the PIMC extracts $G(q)$ from $\chi(q)$ via (1), but it is difficult to determine the large- q LFC because statistical errors in Monte Carlo (MC) data can easily overwhelm the very weak many-body contribution to $\chi(q) - \chi_0(q)$ for $q > 3k_F$. To develop an efficient algorithm for large q , it is desirable to analytically derive the asymptotic properties of $G(q)$ in the large- q limit. In application, this is particularly important since many TDDFT algorithms require an XC kernel $K_{XC}(r)$ in real space, and, without accurate data for large q and analytical forms for $q \rightarrow \infty$, a reliable Fourier transform from $K_{XC}(q)$ to $K_{XC}(r)$ is extremely difficult due to the Gibbs phenomenon.

In this Letter, we develop the VDMC method for the warm dense electron gas, which is a generalization of the method introduced by two of us [39]. Inspired by the binary expression tree in computer science, we introduce an expression-tree representation of Feynman diagrams to efficiently and accurately calculate $\chi(q)$. Our VDMC method is reliable for the UEG of high to intermediate density and at arbitrary temperature, covering those low- T and large- q regimes where other unbiased finite- T quantum MC methods are infeasible. From extensive simulations, we obtain high-precision data of the static LFC in a broad range of (q, T) space from the Fermi liquid to WDM and then to classical plasma. Several interesting physics are revealed, including the T -dependent evolution of the hump structure and the large- q tail (Fig. 1) and the emergence of an asymptotic high- T scaling relation of $G(q; r_s, T)$ (we use a semicolon to separate intrinsic variables including q , ω , and r , and parameter variables including r_s and T) in the dimensionless variable $q/\sqrt{T}$ [Fig. 2(a)]. High-precision data for K_{XC} are obtained up to $14k_F$, shown in Fig. 2(b). In both the small- and the large- q limit, $K_{XC}(q)$ saturates to a constant, nonmonotonically depending on T . Moreover, we show that

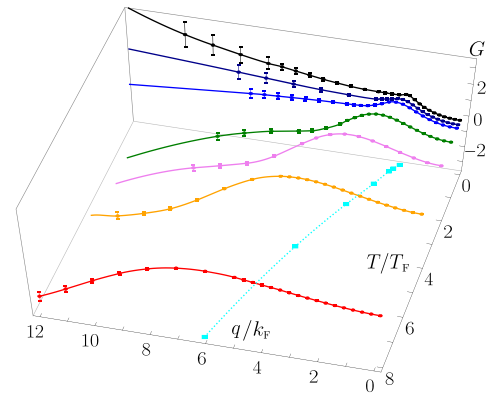


FIG. 1. Static local field correction $G(q)$ in the extensive (q, T) plane for $r_s = 1$. The circles depict VDMC data points for $\theta = 0.0625, 0.25, 0.4, 1, 2, 4, 8$. The cyan squares and dotted line depict the tendency of the maximum momentum $q_{\max}$ of $G(q)$ versus T .

the asymptotic XC kernel $K_\infty \equiv K_{XC}(q \rightarrow \infty)$ is proportional to the interaction-induced shift of the kinetic energy and derive the analytical form of the coefficient. Using a VDMC, we compute the kinetic energy accurately and thus K_∞ as a function of T [the inset of Fig. 2(c)]. Combining data of $K_{XC}(q)$ for $q \leq 14k_F$ and of K_∞ for the tail, we show that the Fourier transform of $K_{XC}(q)$ to real space can be performed reliably without any freely adjustable parameter [Fig. 2(c)].

Results. We carry out extensive simulations for the three-dimensional UEG model at a series of temperatures $\theta = 0.0625, 0.25, 0.4, 1, 2, 4, 8$. Hereby, we focus on parameter $r_s = 1$, which is the most typical WDM density, and we also simulate $r_s = 2$ for $\theta = 4, 8$ to illustrate the r_s -independent scaling relation. We accurately determine the static LFC $G(q; T)$ up to $q/k_F = 14$ (Fig. 1), more than four times larger than the previous studies [46,58]. Accordingly, the XC kernel $K_{XC}(q; T)$ is obtained in Fig. 2(b).

Our data exhibit several profound features of the T - and q -resolved LFC. For any given T , there is a unique momentum $q_{\max}$ corresponding to the local peak in $G(q)$, which separates long-range (small- q) from short-range (large- q) physics. Figure 1 shows that the peak broadens and shifts to the larger momentum as T increases, and the inset of Fig. 2(a) shows $q_{\max}$ as a function of T . In the high- T limit, $q_{\max}$ is controlled by the thermal de Broglie wavelength $\lambda_{th} = \sqrt{4\pi/T}$ as $q_{\max} \approx 7.6\lambda_{th}^{-1}$. As T decreases, the value of $q_{\max}$ gradually decreases and is no longer dominated by λ_{th} for $T \lesssim 2T_F$, eventually converging to $\approx 2k_F$ at zero T . We further observe that in the evolution of the XC kernel $K_{XC}(q)$ with T [Fig. 2(b)], a local minimum appears at $T \lesssim 0.4T_F$ and becomes sharper and closer to $q \approx 2k_F$ as $T \rightarrow 0$. These numerical results confirm the “ $2k_F$ hump” of the ground-state UEG postulated in various theoretical predictions [59–62]. Moreover, the nontrivial T dependence of $q_{\max}$ and the smearing out of the sharp minimum in K_{XC} at $T \sim T_F$ reflect the intense competition between quantum and thermal fluctuations in the WDM regime.

In addition, with increasing T , the large- q LFC evolves from a positive tail at low T to a negative tail for $T \gtrsim 0.4T_F$. Holas [35] predicted the asymptotic behavior $G(q) \propto q^2$ for

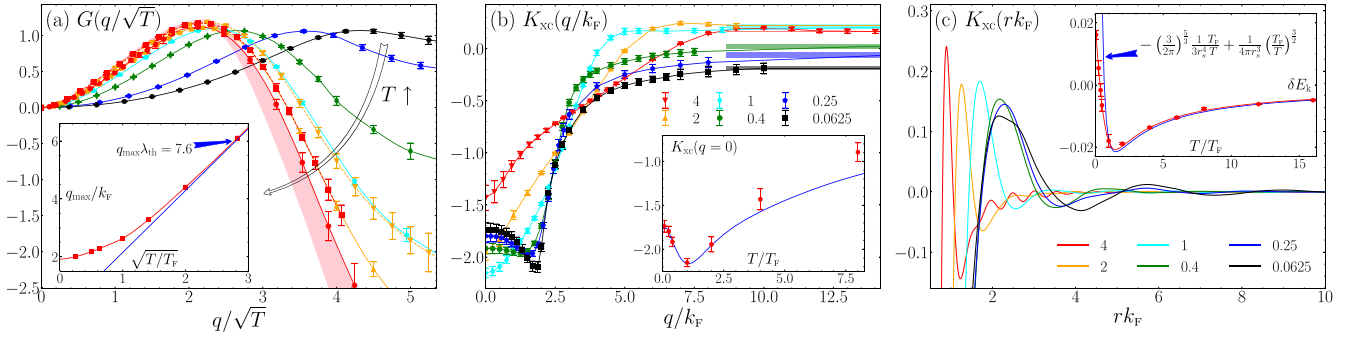


FIG. 2. (a) Rescaled static LFC as a function of $q/\sqrt{T}$. The data points with solid lines are for $r_s = 1$ and $\theta = 0.25, 0.4, 1, 2, 4, 8$, and ones with dashed lines are for $r_s = 2$ and $\theta = 4, 8$. As $T \rightarrow \infty$, the LFC data tend to collapse to a universal curve that depends on $q/\sqrt{T}$, and is covered in the pink shadow. The inset shows the evolution of $q_{\max}$ from $\approx 2k_F$ in the zero- T limit to $\approx 7.6\lambda_{\text{th}}$ in the high- T limit. (b) The XC kernel $K_{\text{xc}}(q)$ for different temperatures and $r_s = 1$. The tail of either curve converges to a constant K_∞ that is explicitly calculated by the VDMC as Eq. (3), and the strip marks its value and error. The inset shows the evolution of $K_{\text{xc}}(q=0, T)$. Our data are consistent with the parametrized function [56] (blue line). (c) The XC kernel of UEG in real space with the delta-peaked term subtracted. The inset shows the interaction-induced shift of the kinetic energy versus temperature. Our data is approaching the high- T approximation [57] (blue line) for $\theta > 1$.

$q \rightarrow \infty$ at zero T , where the prefactor is proportional to the change in the interaction-induced shift of the kinetic energy δE_k and is positive for all r_s . However, no analytical formula currently exists for finite T . Qualitatively, the evolution of the LFC tail reflects the sophisticated competition of Coulomb repulsion, exchange effects, and thermal motion.

We argue that in the high- T limit, the entire LFC curve is described by an asymptotic scaling function depending on a single dimensionless parameter $q/\sqrt{T}$, independent of r_s , as

$$\lim_{T \rightarrow \infty} |_{\text{fixed } \alpha} G(q; r_s, T) = \tilde{G}(\alpha), \quad \alpha = q/\sqrt{T}. \quad (2)$$

The argument is as follows: For UEG, there are two characteristic length scales, i.e., λ_{th} and r_s . When $T \rightarrow \infty$, the only detectable length scale is λ_{th} since $\lambda_{\text{th}} \ll r_s$. Indeed, Fig. 2(a) demonstrates that as T increases, the LFC tends to collapse into a universal curve as Eq. (2).

We now turn to the XC kernel. Figure 2(b) shows that $K_{\text{xc}}(q)$ converges to a nonmonotonic T -dependent constant for both $q \rightarrow 0$ and $q \rightarrow \infty$. It is known that the uniform XC kernel $K_{\text{xc}}(q=0)$ is proportional to the second derivative of the XC free energy, given by the compressibility sum rule [63]. Therefore, we compare our $K_{\text{xc}}(q=0)$ data with the values from the recent XC free-energy parametrization [56] in the inset of Fig. 2(b). It is shown that they are consistent for $\theta \leq 2$ within error bars while having a slight deviation for $\theta \geq 4$.

The large- q behavior of the XC kernel is highly nontrivial, as also discussed in the LFC tail. Based on the large- q expansion of the polarization function Π related to the density response function by $\chi(q, \omega) = [\Pi^{-1}(q, \omega) + v_q]^{-1}$ (details are given in the Supplemental Material [64]), we derive the asymptotic formula of the large- q XC kernel for finite T as

$$\lim_{q \rightarrow \infty} K_{\text{xc}}(q; r_s, T) = K_\infty(r_s, T) + \mathcal{O}(q^{-2}), \quad (3)$$

with $K_\infty = -(32\pi^2 r_s^6 / 27) \delta E_k$. This analytic formula generalizes the zero- T one [35] and describes that the convergent constant K_∞ is controlled by the many-body contributions of the kinetic energy. Note that Eq. (3) still holds for the

dynamic XC kernel since the frequency dependence only exists in the subleading and higher orders. We explicitly calculate the kinetic energies by the VDMC to extract K_∞ for various temperatures, and the results are consistent with our large- q K_{xc} data within error bars, as shown in Fig. 2(b). Furthermore, the inset of Fig. 2(c) displays an interesting nonmonotonic behavior: as T increases, δE_k decreases from a positive value for low T to negative for $\theta \gtrsim 0.4$ and finally approaches zero asymptotically. At zero T , δE_k is always positive because electron repulsion broadens the ground-state momentum distribution. However, at high enough temperatures, the correlation effects would lead to the narrowing of the momentum distribution [57, 65, 66]; meanwhile, the Hartree-Fock term $-(3/2\pi)^{5/3} \theta / (3r_s^4)$ dominates the XC contribution to the kinetic energy so that $\delta E_k < 0$. Remarkably, we find that the high- T approximation [57], including the Hartree-Fock and the Montroll-Ward contributions, describes well the nonmonotonic T dependence of δE_k for $\theta \geq 1$. The formula (3) combined with the behavior of δE_k versus T explains the T -dependent evolution of the LFC/XC kernel tail and matches the scaling relation in the high- T limit.

Combining our numerical data and the analytical tail, we perform interpolation and obtain a controlled representation of the XC kernel for overall momentum [the solid line of Fig. 2(b)]. In practice, we use spline interpolation to fit piecewise cubic polynomials to $q \leq q_{\text{cut}}$ data (the cutoff momentum q_{cut} excludes the tail and depends on the temperature). We then perform the least-squares fits to $q > q_{\text{cut}}$ data via the ansatz $K_{\text{xc}}(q) = K_\infty + a/q^2$, where K_∞ is fixed by δE_k data and a is the fitting parameter. The overall $K_{\text{xc}}(q)$ enables a Fourier transform to the real-space XC kernel $K_{\text{xc}}(r)$ without relying on any ansatz of $K_{\text{xc}}(q)$. The constant tail in $K_{\text{xc}}(q)$ translates to a contact term $K_\infty \delta^{(3)}(r)$ in real space, while the remaining part of the XC kernel transforms into a smooth function of the distance r , as shown in Fig. 2(c). This scheme allows us to accurately represent $K_{\text{xc}}(r)$, which is a key input in TDDFT calculations for real materials.

Methods. Diagrammatic expansion is used to perturbatively calculate a quantity as a series of integrals which can

be visualized as Feynman diagrams. It allows us to simulate quantities immediately in the thermodynamic limit by a Markov-chain process that stochastically samples diagrams and internal variables. Such diagrammatic MC methods have found successful applications in many physical problems [67–92]. For UEG, the expansion in the bare Coulomb interaction is divergent and needs to be transformed into a more appropriate power expansion, as explained below. We use the variational scheme [39,93], in which the emergent low-energy physics is taken into account at the lowest order, and the corrections are perturbatively added, leading to rapid convergence. We develop a VDMC method, which has a generic algorithmic structure and an optimized efficiency with the help of an expression-tree representation of diagrams.

Motivated by the Coulomb screening effects, we introduce a variational inverse screening length λ_q following Ref. [39] to reexpand the bare interaction $\frac{8\pi}{k^2} = \frac{8\pi}{k^2 + \lambda_q^2} \sum_{n=0}^{\infty} \left(\frac{\lambda_q^2}{8\pi} \frac{8\pi}{k^2 + \lambda_q^2} \right)^n$. In the VDMC, λ_q is q dependent and optimized to achieve a rapid convergence according to the principle of minimal sensitivity [94]. To further speed up the convergence, we insert the Fock subdiagram into the bare electron propagator to recover the screened Hartree-Fock approximation in the first order. Meanwhile, we add order-by-order chemical-potential counterterms to fix the Fermi surface at each order. Within this optimized expansion, we can obtain reliable infinite-order results of arbitrary quantities without very large truncation order N , which avoids the exponential scaling of the computation time with order. Figure 3(a) shows the static polarization $\Pi(q)$, which rapidly converges at the optimal λ_q . In practical simulations, we choose λ_q as piecewise constants for $q \lesssim 6k_F$ and $q \gtrsim 6k_F$, which is already sufficient for rapid convergence. We compute the Feynman diagrams up to order $N = 5$, which contain about 1200 diagrams. Our calculations suggest that, at least for UEG, $N = 5$ is already sufficient for us to reliably extrapolate $\Pi(q)$ to infinite order. The description of details, including the topology and number of Feynman diagrams and numerical approach, can be found in Ref. [39].

A major challenge of the VDMC is how to generate and group a large number of Feynman diagrams and efficiently compute their weights. By sign-structure analysis of scattering amplitudes in diagrams constrained by the crossing symmetry and the conservation law [95], we can optimize the internal-variable arrangements and construct the sign-canceled diagram groups to alleviate the sign problem significantly. Inspired by the binary expression tree in data structures, we develop a universal expression-tree representation of diagrams implemented by a diagram minicompiler with a three-layer infrastructure. We are improving the original code for readability and usability and will report details elsewhere.

By the VDMC method, we obtain more accurate LFC data over a wider range of (q, T) than the state-of-the-art PIMC [46], as shown in Fig. 3(b). We note that for the LFC at large momenta, the PIMC cannot provide reliable results because the statistical errors of data of χ ($\sim 1/q^2$) overwhelm

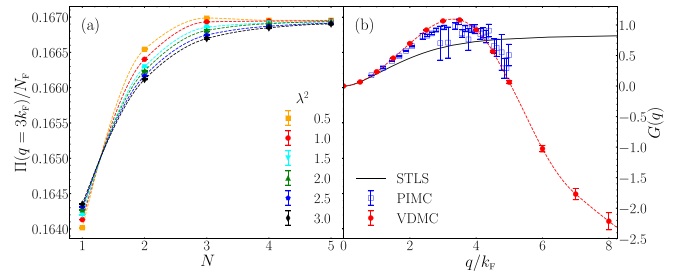


FIG. 3. (a) Static polarization scaled by the density of states at the Fermi level N_F at $q = 3k_F$ versus truncation order N for $\theta = 2$ and $r_s = 1$. All λ choices lead to the same extrapolated value, and the optimal λ for the fastest convergence is about 1.0 in this case. (b) LFC $G(q)$ at $\theta = 2$ and $r_s = 1$ for the VDMC (red circles), the PIMC [46] (blue squares), and the finite-temperature version [96] of the STLS approximation [97] (black line). The STLS approximation is a widely used self-consistent scheme for an approximate treatment of the static LFC.

$\chi - \chi_0$ ($\sim 1/q^4$) [64]. Here, based on the large- q expansion of $\chi(q)$ [64], we identify each polarization diagram with a tail-decaying behavior $q^{-\ell}$, where ℓ is the least number of the propagator lines with flowing q . Hence, we optimally organize the external momentum variable of each diagram to make the integrand have the same tail behavior as the integral so that the VDMC can directly calculate $\chi - \chi_0$ by efficiently sampling each diagram with a reweighting factor q^ℓ . For completeness, we mention that a VDMC simulation for a single $r_s - \theta$ system parameter takes $O(10^4)$ CPU (single-threaded process) hours.

Discussion. In summary, we present a systematic and generic VDMC approach for warm dense electron gas and obtain high-precision results for the LFC/XC kernel over a broad range of momentum and temperature. The VDMC allows for accurate and efficient calculation of various quantities directly in the thermodynamic limit at arbitrary temperature, beyond the reach of state-of-the-art path-integral-based MC methods. Our VDMC calculations have immediate practical applications in exploring various physical systems. For example, we obtain the first *ab initio* result for the real-space XC kernel, which enables finite- T TDDFT calculations for real electronic systems. A natural continuation of this work is to study the spin-dependent correlations and thermodynamic functions and construct the frequency-dependent LFC.

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