

Estimates of the dynamic structure factor for the finite temperature electron liquid via analytic continuation of path integral Monte Carlo data

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Understanding the dynamic properties of uniform electron gas (UEG) is important for numerous applications ranging from semiconductor physics to exotic warm dense matter. In this work, we apply the maximum entropy method (MEM), as implemented by Thomas Chuna *et al.*, *J. Phys. A Math. Theor.* **58**, 335203 (2025), to *ab initio* path integral Monte Carlo (PIMC) results for the imaginary-time correlation function $F(q, \tau)$ to estimate the dynamic structure factor $S(q, \omega)$ over an unprecedented range of densities at the electronic Fermi temperature. To conduct the MEM, we propose to construct the Bayesian prior μ from the PIMC data. Constructing the static approximation leads to a drastic improvement in $S(q, \omega)$ estimate over using the simpler random phase approximation (RPA) as the Bayesian prior. We present results for the strongly coupled electron liquid regime with $r_s = 50, \dots, 200$, which reveal a pronounced roton-type feature and an incipient double peak structure in $S(q, \omega)$ for intermediate wave numbers at $r_s = 200$. We also find that our dynamic structure factors satisfy known sum rules, even though these sum rules are not enforced explicitly. To verify our results, we show that our MEM estimates converge to the RPA limit at higher densities and weaker coupling $r_s = 2$ and 5. Further, we compare with two different existing results at intermediate density and coupling strength $r_s = 10$ and 20, and we find good agreement with more conservative estimates. Combining all of our results for $r_s = 2, 5, 10, 20, 50, 100, 200$, we present estimates of a dispersion relation that show a continuous deepening of its minimum value at higher coupling. An advantage of our setup is that it is not specific to the UEG, thereby opening up new avenues to study the dynamics of real warm dense matter systems based on cutting-edge PIMC simulations in future works.

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I. INTRODUCTION

Uniform electron gas (UEG) is an important and well-studied physical system [1–5]. Investigations on this topic have continued for decades because there is no closed analytic model that can describe the spatial and temporal structure of the plasma at all experimentally accessible number densities and temperatures. A current frontier of UEG is the finite temperature electron liquid, where the plasma is both quantum degenerate, $\Theta = k_B T / E_F \approx 1$, and strongly coupled, $\Gamma = \frac{1}{r_s} [(k_B T)^2 + E_F^2]^{-1/2} \geq 1$. We have adopted Hartree atomic units in this work, with r_s being the Wigner-Seitz radius that is defined by $n_e = (4\pi r_s^3/3)^{-1}$ (in units of Bohr radius a_B), E_F is the Fermi energy in Hartree, and $\beta = (k_B T)^{-1}$ is the inverse temperature. When the plasma is both quantum degenerate and strongly coupled, path integral Monte Carlo (PIMC) simulations are one of the few methods that can describe

the structure of the UEG [6]. In this work, we study PIMC simulations of the electron liquid at fixed $\Theta = 1$ and vary Γ between approximately 1 and 150; this gives us access to a broad range of physical conditions.

In principle, PIMC simulations give one access to the complete equilibrium dynamics of the simulated system in the form of various imaginary-time correlation functions (ITCFs) [7–9]. In particular, the imaginary-time density-density correlation function $F(q, \tau) = \langle \hat{n}(q, \tau) \hat{n}(-q, 0) \rangle$, which corresponds to the usual intermediate scattering function evaluated at the imaginary time argument $t = -i\hbar\tau$, with $\tau \in [0, \beta]$ and $\beta = 1/k_B T$ the inverse temperature in energy units, is directly related to the dynamic structure factor (DSF) $S(q, \omega)$ (in units of inverse energy) via a two-sided Laplace transform

$$F(q, \tau) = \int_{-\infty}^{\infty} d\omega e^{-\tau\omega} S(q, \omega) \quad (1a)$$

$$= \int_0^{\infty} d\omega (e^{-\tau\omega} + e^{-(\beta-\tau)\omega}) S(q, \omega), \quad (1b)$$

where the second equality follows from the detailed balance condition $S(q, -\omega) = S(q, \omega)e^{-\beta\omega}$. Matching β, ω is the frequency in energy units. Since the left-hand side (LHS) is a function of imaginary-time and the right-hand side (RHS) is a function of real-time frequency, estimating the DSF is an

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analytic continuation problem. The DSF is of key importance, e.g., for the interpretation of x-ray Thomson scattering experiments [10–12], and directly gives one access to a number of density response and dielectric properties [13,14]. Unfortunately, inverting (1) to reconstruct $S(q, \omega)$ from $F(q, \tau)$ is a well-known exponentially ill-posed problem [15,16] and plagues many fields of science [17–26].

For UEG, Dornheim *et al.* [27–29] attempted this problem by evoking the fluctuation–dissipation theorem, which has allowed us to exactly fulfill a number of exact constraints that are known for UEG. However, this *stochastic sampling* approach breaks down with increasing coupling strength, and cannot be easily generalized to real systems beyond the UEG model. Also for the UEG, Filinov *et al.* [30] have attempted this problem by evoking the Nevanlinna transformation of the inverse dielectric function (IDF), which is trivially related to the DSF. To give the flexibility needed to fit the data, the authors express the five-moment Nevanlinna function in terms of the nine-moment Nevanlinna function and fit the additional moments. However, the DSF estimate is a nonlinear function of the data, and resampling techniques are needed to propagate the uncertainty in the data to the final estimates [31]. This is not done, however, thus the error estimates may be underestimated. Also, applying the Nevanlinna approach to multicomponent systems may prove challenging because in two-component systems only clever constructions allow a subclass of Nevanlinna functions to possess five convergent moments, let alone nine (see Ref. [32], Sec. III A 1). Compared to either the stochastic or Nevanlinna approaches, the MEM is agnostic to the underlying system, and it can be applied directly to two-component systems that are comprised of both electrons and nuclei.

The recent work of Chuna *et al.* [33] has demonstrated that the all-purpose maximum entropy method (MEM) can reliably estimate the DSF from UEG PIMC data at $r_s = 10$, $\Theta = 1$. Specifically, Bryan’s MEM produces visually identical estimates to the dual Newton MEM and thus does not overregularize. In the present work, we apply the MEM with Bryan’s optimization algorithm to estimate the UEG DSF at $\Theta = 1$ over a broad range of densities identified by the corresponding Wigner-Seitz radius. In particular, we investigate densities spanning the warm dense matter regime [34] ($r_s = 2$) to the strongly coupled electron liquid [35–37] ($r_s = 50, \dots, 200$). We compare our estimates with the more limited stochastic inversion where it is available, i.e., for $r_s \leq 10$. As we apply the MEM, we have given special attention to our uncertainty procedure. The MEM requires ITCF data and a best guess of the solution (i.e., Bayesian prior). In our application, we construct the Bayesian prior directly from the ITCF data based on the *static approximation* to the DSF that approximates the full dynamic local field correction (LFC) by its exact static limit, i.e., $G(q, \omega) \approx G(q, 0)$. The static approximation has been shown, in many finite temperature electron liquid applications, to yield a good approximation of the DSF [27,28,38]. We consider the impact of using such a Bayesian prior that depends on the data, and we compare the static approximation to the simpler random phase approximation (RPA) that neglects the LFC entirely. In addition to this, we quantify the uncertainty in our DSF estimates via leave-one-out

binning [31,39,40], which estimates the variance arising from uncertainty in the MEM regularization weight and from sampling error in the two-particle correlation function.

Thus, this work establishes how to use the general purpose tool, the MEM, to estimate the UEG DSF from PIMC data for the ITCF. In the weak-coupling limit $\Gamma \rightarrow 0$, our estimates resemble the RPA, as expected. In addition, our estimates match results obtained by stochastically sampling the dynamic local field corrections [27] for $r_s \leq 10$, and our setup works well even at large r_s where the latter approach fails. We find a pronounced roton-type feature in our new estimates for $S(q, \omega)$ at intermediate wave numbers q that emerges with increasing coupling strength. This feature has been observed in a number of recent theoretical studies of strongly correlated quantum Coulomb systems [30,41–44] and phenomenologically resembles the roton feature reported in both fermionic He-3 [45,46], bosonic He-4 quantum liquids [47,48], and dusty plasmas [49,50]. Our estimates also show an incipient double peak structure, which emerges at strong coupling and matches strongly coupled molecular dynamics simulations [51,52] and investigations of the UEG [30,44,53]. Finally, our estimates recover the appropriate sum rule behaviors, even though the sum rules are not explicitly enforced on the solution as a constraint.

There are many future applications of the DSFs estimated in this work; we name only a few here. First, determining the full frequency dependence of the dynamic LFC $G(q, \omega)$ provides an estimate for a nonadiabatic dynamic exchange-correlation kernel for linear response time-dependent density functional theory (TD-DFT) [54–56]. Such kernels would inform simulations of a host of dynamic and transport properties of real multicomponent systems, and we expect that an improved treatment of dynamic exchange-correlation effects might be particularly important to study electron-electron effects such as the roton mode that has recently been predicted to occur in warm dense hydrogen [41]. Second, the estimated DSF is related to various dielectric and transport properties via Kramers-Kronig relations or sum rules [3,13,14,57,58]. Third, the DSF of the UEG is important for the interpretation of x-ray Thomson scattering experiments within the widely used Chihara decomposition [10,11,59]. Finally, these estimated DSFs establish a benchmark for new dynamic theories in the strongly coupled regime, such as (non)equilibrium Green’s functions [60–62] and dynamic dielectric theories [37,63,64].

The remainder of this paper is organized as follows: In Sec. II, we discuss methods. We give a short review of the MEM, discuss the static LFC and the RPA, contemplate the implications of using the data twice (i.e., first to estimate the Bayesian prior and second to conduct the MEM), and finally we describe the leave-one-out uncertainty quantification procedure. In Sec. III, we present our comparison to the RPA at $r_s = 2, 5$, our comparison to the stochastic estimates at $r_s = 10$, our comparison to Nevanlinna estimates at $r_s = 20$, our new strong coupling results at $r_s = 50, 100, 200$, we examine the dispersion relations across all r_s , and finally we demonstrate that certain sum rules are satisfied even though they are not enforced by the MEM. In Sec. IV, we draw conclusions from our results. We also provide substantial Appendices. In Appendix A, we derive the inverse sum rule and show that the static approximation must satisfy this rule. In Appendix B,

TABLE I. Tabulation of the physical parameters describing the path integral Monte Carlo simulations used in this work. We list the quantum degeneracy parameter $\Theta = k_B T / E_F$, the coupling parameter $\Gamma = \frac{1}{r_s} ((k_B T)^2 + E_F^2)^{-1/2}$, the Fermi wave number k_F , the plasma frequency $\omega_{p,e}$, the inverse temperature β in units of energy, the number of particles in the simulation, the volume of the simulation (i.e., the length of the periodic boundary cubed), the independent seeds (i.e., the number of independent MCMC simulations), and the typical error in the ITCF values $O[\delta F]$ obtained using Hatano's error analysis [102]. Note that ITCF values are of the order 1, so $O[\delta F]$ is also indicative of the relative error.

r_s	2	5	10	20	50	100	200
Θ	1	1	1	1	1	1	1
Γ	1.54	3.84	7.68	15.4	38.4	76.8	154
k_F (1/Bohr)	9.596×10^{-1}	3.838×10^{-1}	1.919×10^{-1}	9.596×10^{-2}	3.838×10^{-2}	1.919×10^{-2}	9.596×10^{-3}
$\omega_{p,e}$ (Hartree)	6.124×10^{-1}	1.549×10^{-1}	5.477×10^{-2}	1.936×10^{-2}	4.899×10^{-3}	1.732×10^{-3}	6.124×10^{-4}
β (Hartree)	2.172×10^0	1.358×10^1	5.430×10^1	2.172×10^2	1.357×10^3	5.430×10^3	2.172×10^4
particles	34	34	34	34	34	34	34
volume (cm ³)	1.69×10^{-22}	2.64×10^{-21}	2.11×10^{-20}	1.69×10^{-19}	2.64×10^{-18}	2.11×10^{-17}	1.69×10^{-16}
ind. seeds	1000	1000	1000	1000	1000	1000	1000
$O[\delta F]$	10^{-3}	10^{-3}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}

we provide heatmaps of the relative error across all r_s that shows systematic ringing that is common for entropic regularization. In Appendix C, we provide a complete collection of heatmaps, supplementing $r_s = 50, 100, 200$ from the main text with $r_s = 2, 5, 10, 20$. In Appendix D, we provide cross sections for all r_s . In Appendix E, we verify that the sum rules are satisfied at all r_s , providing sum rule plots for all r_s .

II. METHODS

A. Maximum entropy method via Bryan's algorithm

In this work, we use the all-purpose MEM to estimate the DSF by inverting Eq. (1), which has been used in many other cases [24,65,66]. We supply two practical considerations that support this choice. The MEM has a large literature base to make practitioners familiar with the approach, and many investigations establish the systematics of the MEM. In particular, entropic regularizers tend to contain ringing in the solution [67], and among entropic regularizers the MEM tends to be the smoothest [23,26]. The second reason is that it allows for a rigorous error analysis. The MEM quantifies the uncertainty arising from the regularization weight [65], and it is computationally cheaper than other methods [23], so it can be used in a resampling procedure to estimate the uncertainty arising from the data.

Many thorough reviews of the MEM exist [24,65]. The MEM relies on a Bayesian framework created by Gull [68], which shows how to average over a collection of solutions produced by solving the optimization problem (2) at different regularization weights α ,

$$\max_x -\frac{1}{2} \|Ax - b\|_C + \alpha S_{\text{SJ}}[x | \mu]. \quad (2)$$

Here $\|Ax - b\|_C = (Ax - b)^T C^{-1} (Ax - b)$ is the generalized least squares criterion, and $S_{\text{SJ}}[x | \mu] = \sum_i x_j - \mu_j - x_j \ln x_j / \mu_j$ is the Shannon-Jaynes (SJ) relative entropy regularizer. For this problem, we have the matrix $A_{i,j} = \exp(-\tau_i \omega_j) + \exp(-(\beta - \tau_i) \omega_j)$, the data vector $b_i = F(q, \tau_i)$, the error of the data,

$$C_{ij}^{\text{bin}0} = \frac{\sigma_{F^{\text{bin}0}}^2}{\sqrt{N-1}} \delta_{ij}, \quad (3)$$

the Bayesian prior μ_j , and the desired solution vector $x_j = S(q, \omega_j)$ all at fixed wave number q . From the collection of solutions obtained varying α , the MEM yields an estimate of the solution and the uncertainty arising from the choice of α . We estimate 50 α solutions, sampling logarithmically from 10^{-3} to 10^7 . Here we resolve a uniformly sampled frequency domain $[\omega_{j=0}, \omega_{j=\text{max}}]$, with grid spacing $\Delta\omega = 0.02\omega_{p,e}$. The max value is determined for a given q as the first index such that the Bayesian prior is 10^{-14} smaller than its peak value, i.e., $\mu_j < 10^{-14} \max_j \{\mu_j\}$.

We rely on Bryan's algorithm to solve Eq. (2) at these α values [69], even though Bryan's algorithm only approximates the solution to (2) [33,69,70]. We do this because Chuna *et al.* [33] proposed a dual Newton algorithm that does not make approximations, and yet when the noise is small, as is the case for these data (see Table I), Bryan's algorithm performs comparably to its alternative. The numeric implementation of either approach is freely available in Ref. [71].

B. Choice of Bayesian prior μ

1. Models of the finite temperature electron liquid dynamic structure factor

Early models of the dynamic response of one-component plasmas were developed for either classical or quantum weakly coupled systems [72–75], $\Gamma \ll 1$, meaning that only the self-interaction energy was accounted for [76,77]. Later models were developed for the dynamic response in classical strongly coupled systems [78,79], $\Gamma \geq 1$, meaning that N -body correlation effects were also being taken into account. However, the finite temperature electron liquid is both strongly coupled and quantum degenerate, $\Theta \approx 1$. Thus, N -body exchange effects are important as well. In selecting a suitable default model for the Bayesian prior, we consider the random phase approximation, which is accurate in the high-density limit where the UEG is weakly coupled. In addition, we consider a second, vastly improved default model for the Bayesian prior that takes into account PIMC results for exchange-correlation effects on the static level.

The DSF is related to the system's dynamic linear density response function $\chi(q, \omega)$, where q and ω are the wave number and frequency of a weak external harmonic perturbation

[12], via the fluctuation dissipation theorem [1],

$$S(q, \omega) = -\frac{1}{\pi n} \frac{\text{Im}\chi(q, \omega)}{1 - e^{-\beta\hbar\omega}}. \quad (4)$$

Without loss of generality, the density response is often expressed as [58,72,79]

$$\chi(q, \omega) = \frac{\chi^0(q, \omega)}{1 - v(q)[1 - G(q, \omega)]\chi^0(q, \omega)}. \quad (5)$$

Here $v(q)$ is the Coulomb interaction and $\chi^0(q, \omega)$ describes the density response of the noninteracting Fermi gas at finite temperatures. For our implementation of $\chi^0(q, \omega)$, we relied on Giuliani and Vignale's textbook [1] as well as the work by Tolias *et al.* [64]. Kugler indicates a few $q \rightarrow 0$ sanity checks that we verified as well [80].

The dynamic local field correction $G(q, \omega)$ in (5) contains the full wave number and frequency resolved information about exchange-correlation effects. It is formally related to the dynamic exchange correlation kernel from linear response time-dependent density functional theory [81,82]. Therefore, $G(q, \omega)$ modifies the interaction potential such that the exchange and correlation effects are included, in which case this seemingly one-body description includes all the N -body physics [83]. The random phase approximation corresponds to $G(q, \omega) \equiv 0$ and, thus, describes the dynamic density response on the mean-field level, neglecting exchange-correlation effects. In contrast, the static approximation only neglects the dynamic effects by setting $G(q, \omega) \approx G(q, 0)$ [84,85].

In the context of the present work, the foremost advantage of the static approximation is that $G(q, \omega = 0)$ is computed directly from the PIMC data, avoiding the problematic and arbitrary selection of a model that is only valid in a certain density and temperature limit. The procedure for constructing the static LFC is given, e.g., in Ref. [38]; we do not use the neural network representation reported therein, as it has only been trained for $r_s \leq 20$ [38]. Instead, before conducting the analytic continuation, we compute the static LFC $G(q, \omega = 0)$, and we construct the Bayesian prior. The formula to calculate $G(q, \omega = 0)$ from the PIMC data is obtained by inverting (5) and setting $\omega = 0$. The unknown $\chi(q, \omega = 0)$ can be estimated from the data via the imaginary time version of the fluctuation dissipation theorem

$$\frac{\chi(q, \omega = 0)}{n\beta} = -\frac{1}{\beta} \int_0^\beta d\tau F(q, \tau), \quad (6)$$

derived, e.g., in the Appendix of Ref. [86].

Many investigations have been conducted comparing the RPA and the static approximation for the UEG [27,28,87]. Both the RPA and the static approximation exhibit a single sharp peak at the plasma frequency at small q , where the effect of $G(q, 0) \sim q^2$ vanishes. Conversely, $v(q)G(q, \omega = 0)$ becomes constant at large q [88] (i.e., small length scales $\lambda = 2\pi/q$), and its effects on the dispersion relation vanish. The discrepancies between the RPA and static approximation occur where the wavelength λ is roughly the interparticle spacing $2\pi/q \approx r_s$, and they are explained by the electron pair alignment model [42]. The authors argue that density fluctuations caused by an external perturbation of wavelength

$2\pi/q \approx r_s$ need less energy compared to other density fluctuations because this wave number coincides with a spatial pattern that minimizes the potential energy of the system. Since the potential energy of the system is dependent on the exchange-correlation interaction energy and RPA entirely neglects these effects, the static approximation will greatly differ from the RPA in this region. Further, since exchange-correlation effects become more important with increasing coupling, this disagreement becomes more pronounced with increasing r_s .

Investigations have found that the static approximation exhibits a negative dispersion relation (i.e., roton feature) [27,30,41–44], satisfies the small- q limit for $S(q)$ [89], violates the large- q asymptotic convergence for $S(q)$ [87,90,91], and empirically satisfies the frequency sum rule (i.e., F-sum rule) and higher sum rules [86,92,93]. Further, investigation has also seen that the inverse moment sum rule is satisfied [89]; we provide an analytical proof for the latter in Appendix A.

Lastly, going beyond the static approximation, investigations have shown that including the dynamic dependence in the local field correction corrects the large- q limit for $S(q)$ [91], enhances the roton feature [27], and creates an incipient double peak structure [42], or in some investigations a second stronger peak [30]. A double peak structure, which results from dynamic LFCs, can be understood as an excitonic effect and has been documented [30,43,44,53,94]. In summary, the static LFC has a record of including much of the important physics, but by definition it does not include the full dynamics dependencies desired in a DSF model.

2. Discussion of extracting the Bayesian prior from the data

Using the data to extract both the Bayesian prior and the final DSF estimate is less *ad hoc* than more traditional Bayesian priors; this is expected to mitigate the bias introduced by the choice of the Bayesian prior. Other works have encouraged using the moments of the data to construct an improved default model [24,95,96] or using stochastic optimization [19], but these works do not consider complications that may arise in uncertainty quantification. So in the following text, we contemplate our approach.

We argue that our method of extracting the Bayesian prior is comparable to common data detrending approaches seen in data science [97]. Examples of detrending can be found in introductory textbooks [40,98,99]; SciPy Signal library's even has a built-in detrend function [100]. Detrending identifies and removes the easily spotted trends in the data before beginning data analysis procedures; this focuses the algorithm's inference capability on the parts of the data that are poorly understood. A simple example of this is known to all scientific fields. When analyzing probabilistic samples, we first center the samples about the sample mean and then scale the samples by the sample's standard deviation. In the case of this analytic continuation algorithm, we are doing something only slightly more sophisticated than centering the data and standardizing the data. Equation (6) has the form of the mean value theorem from introductory calculus. Thus, $\frac{\chi(q, \omega=0)}{n\beta}$ is the average value of the ITCF. In this sense, the static LFC is informing our default model of the data's mean value, so that the inference

power is not wasted on resolving the mean. To relate this discussion to the physics presented in Sec. II B 1, we are doing some initial work so that the MEM is only extracting the dynamic corrections to the static approximations.

From a statistics perspective, we argue that extracting the Bayesian prior from the data reduces the bias introduced in entropic regularization. In statistical inference, regularization is introduced to produce a better estimator. Regularization introduces a bias to reduce the estimator's sensitivity to the data. This is known as the bias-variance tradeoff [40]. Both the choice of regularizer and, if the regularizer includes a Bayesian prior, the choice of Bayesian prior introduce bias. Axiomatic arguments conclude that, unlike other regularizers, entropic regularization does not introduce spurious correlations in $S(q, \omega)$ across ω [24]. Thus, our primary concern is the choice of Bayesian prior. In the discussion of possible Bayesian priors (see Sec. II B 1), we established that $G(q, \omega)$ determines the prior. In fact, determining $G(q, \omega)$ is equivalent to solving the analytic continuation problem [28]. Clearly, choosing $G(q, \omega) = 0$ introduces a bias. By comparison, the static approximation will recover $G(q, \omega) = 0$ where it is reasonable, but can deviate from this value. This suggests that the bias arising from using the static approximation can be no worse than the RPA. Maybe a $G(q, \omega)$ that does not neglect the ω -dependence can be computed to further reduce the bias of the static approximation, but as stated, determining the dynamic dependencies is equivalent to solving the problem. So this becomes a *chicken-and-egg* problem. This suggests that the static approximation is an optimal balance of reducing bias without *a priori* knowing the true solution. To relate this discussion to the physics presented in Sec. II B 1, the static LFC $G(q, \omega = 0)$ can be obtained cheaply from the data to create a Bayesian prior that has less bias than the RPA.

Next we consider Stein's paradox, a statistical concern [101]. Stein's paradox examines how to estimate quantities from data. The general idea is communicated by a simple example. Consider a set of M Gaussian distributed quantities ($a, b, c, \dots, m$) that you sample N times (i.e., $a_0, \dots, a_{N-1}$). If you want to estimate the center of the Gaussian distribution ($\langle a \rangle, \langle b \rangle, \langle c \rangle, \dots$), then taking the average of all the a 's, b 's, c 's individually is *not* the best way to do this. Instead, Stein's estimator dominates this naive approach when $M \geq 3$. In general, Stein's paradox and later proofs are a warning that if the error of every parameter is important, then a combined fit is the best way to get the lowest total error. Assuming that Stein's paradox applies, then it informs us that if we estimated our Bayesian prior and MEM solution simultaneously, we may be able to concoct an estimator that improves the combined error. However, we are only focused on producing the best MEM estimate, the Bayesian prior is only a concern in that it effects this estimate. To relate this discussion to the physics presented in Sec. II B 1, we are not concerned with the accuracy of the static approximation because we know it is wrong. Hence we do not make efforts to improve the estimate.

The only remaining concern given the discussions above is the general concern of how the error in the default model propagates into the MEM estimate, which would apply to any Bayesian prior we select; leave-one-out binning can quantify such error.

C. Leave-one-out binning

To estimate both the DSF and its related statistical uncertainty from the PIMC data for $F(q, \tau)$, we use the leave-one-out binning over independent PIMC simulations. This procedure is also known as jackknife binning [31, 39, 40]. We are motivated to use leave-one-out-binning procedure for two reasons. First, we need an uncertainty quantification tool that can include uncertainty arising from estimating the Bayesian prior from the data. Second, we need a tool that can handle biased nonlinear error estimates (note that the entropic regularization makes the MEM, itself, a biased nonlinear function acting on the data to produce a DSF estimate). Based on Berg [39], leave-one-out binning is the simplest tool we can expect to handle both issues.

Leave-one-out-binning is a resampling algorithm that produces N estimates from N independent samples by creating N subsets of the data, known as bins. As the name indicates, the zeroth subset of data, known as bin 0, leaves out data sample 0 (i.e., contains samples $1, \dots, N-1$). For this bin, we estimate the ITCF $F^{\text{bin}0}$ and the error $C_{ij}^{\text{bin}0}$ using Hatano's error analysis [102]. With this bin's ITCF, we construct a Bayesian prior $\mu^{\text{bin}0}$ by computing $G(q, \omega = 0)$ and (6). Then we use both the Bayesian prior and ITCF together to solve (2) at a collection of α 's. In total, this procedure yields, for each bin, an unparametrized estimate of the DSF $S(q, \omega)_{\text{bin}}$, the uncertainty with respect to α $\text{Var}_\alpha S(q, \omega)_{\text{bin}}$, and the MEM posterior weighting function.

Using the outputs of the leave-one-out-binning procedure, we can estimate the variance in the solution with respect to perturbations in the data δF as

$$\text{Var}_{\delta F}[S(q, \omega)] = \sum_{\text{bins}} [\langle S(q, \omega) \rangle - S(q, \omega)_{\text{bin}}]^2. \quad (7)$$

We can also estimate the variance in the solution with respect to regularization weight α as

$$\text{Var}_\alpha[S(q, \omega)] = \frac{1}{N} \sum_{\text{bins}} \text{Var}_\alpha[S(q, \omega)_{\text{bin}}]. \quad (8)$$

We find that the variance in the estimate across bins is of the same order of magnitude as the variance in the estimate across α . So both statistical and regularization uncertainty are important. To investigate the correlations between statistical uncertainty and α uncertainty, we looked at the collection of MEM posterior weighting functions, finding that they varied little across bins. We concluded that the α uncertainty was not sensitive to perturbations in b . Due to this insensitivity, we added the uncertainties in quadrature,

$$\delta S(q, \omega) = \sqrt{\text{Var}_\alpha[S(q, \omega)] + \text{Var}_{\delta F}[S(q, \omega)]}. \quad (9)$$

Heatmaps of the error $\delta S(q, \omega)$ across q and ω for different r_s values are presented in Appendix B.

III. RESULTS

A. Description of data and data storage

In this section, we present the estimated DSFs obtained using the methods discussed in Sec. II on the PIMC simulation data described in Table I. Our PIMC data contain $M = 1000$ independent runs, generated via the open-source ISHTAR code

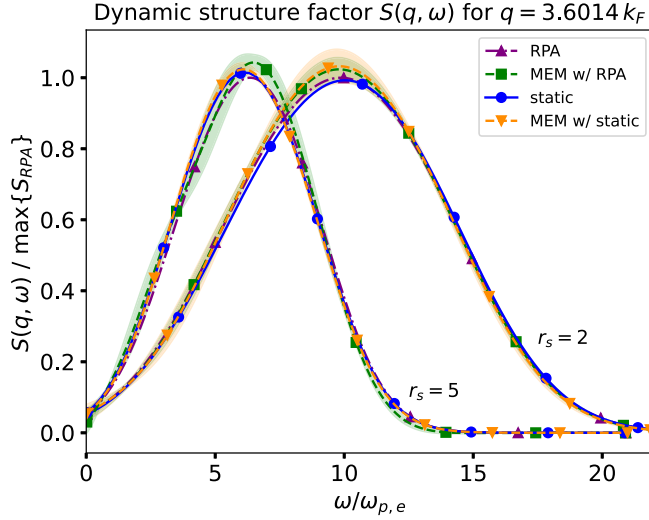


FIG. 1. Plots of $S(q, \omega)$ at $q = 3.6013 k_F$ for both $r_s = 2$ and 5 . The legend indicates which colors/symbols correspond to the MEM estimate and its associated Bayesian prior. For a given r_s value, all of the curves heavily overlap, and the associated r_s value is indicated by a nearby text placement.

[103], which is a canonical implementation [104] of the worm algorithm by Boninsegni *et al.* [105,106]. The error analysis on these data must account for the fermion cancellation problem (i.e., sign problem); we use Hatano's procedure [102], which efficiently deals with the underlying ratio estimation. From Table I, the typical uncertainty in the ITCF values decreases with r_s , where the UEG behavior is well-understood. The leave-one-out binned ITCFs and the MEM estimates of $S(q, \omega)$ are both freely available [107].

B. Validation of MEM estimates at weak and intermediate coupling

1. Comparison to RPA at weak coupling

For $r_s = 2$, $\Gamma = 1.54$ and $r_s = 5$, $\Gamma = 3.84$, the static LFC and RPA DSFs are similar; unsurprisingly, the resulting MEM estimates are similar. This demonstrates a desirable

insensitivity to the prior. A single example is demonstrated for $q = 3.6013 k_F$ in Fig. 1. Similar quality results exist for all q , and the interested reader may check Appendix C for heatmaps and Appendix D for q cross sections from those heatmaps.

2. Comparison to the stochastic approach at intermediate coupling

As mentioned in the Introduction, a stochastic sampling algorithm has already been employed for $r_s = 10$, $\Theta = 1$ UEG PIMC data in Refs. [27,29]. This approach is specific to the UEG, for which it automatically fulfills a number of exact constraints and sum rules. By comparison, the MEM has no guarantee of satisfying sum rules. In Fig. 2, we compare our DSF estimates to these stochastic estimates because we expect that the general shape of the stochastic estimate is physical and provides information through comparison even if the stochastic estimate is not the exact inversion either. We find good qualitative agreement in the shape and quantitative agreement in the peak position. Further, Chuna *et al.* [108] demonstrated that these MEM estimates yield three orders of magnitude smaller deviations from the data (i.e., smaller χ^2) than the stochastic estimate.

3. Comparison to the Nevanlinna approach at intermediate coupling

As mentioned in the Introduction, Filinov *et al.* [30] conduct the analytic continuation for $r_s \leq 36$ using the Nevanlinna transformation. Filinov *et al.* set some of the Nevanlinna function's parameters by enforcing behavior with respect to the static structure factor and the static density response. The free parameters are set via either the SHAN or 9MA approach. The SHAN approach maximizes the Shannon-Jaynes entropy with no (i.e., flat) Bayesian prior. The 9MA enhances this by initializing to the SHAN free parameters and then stochastically optimizing according to the goodness-of-fit (10). Filinov *et al.* emphasize that results for either the SHAN or 9MA approach match the data within the statistical error bars, and so a unique DSF is unknown, but they also emphasize that the 9MA, as expected, performs better according to their goodness-of-fit (10).

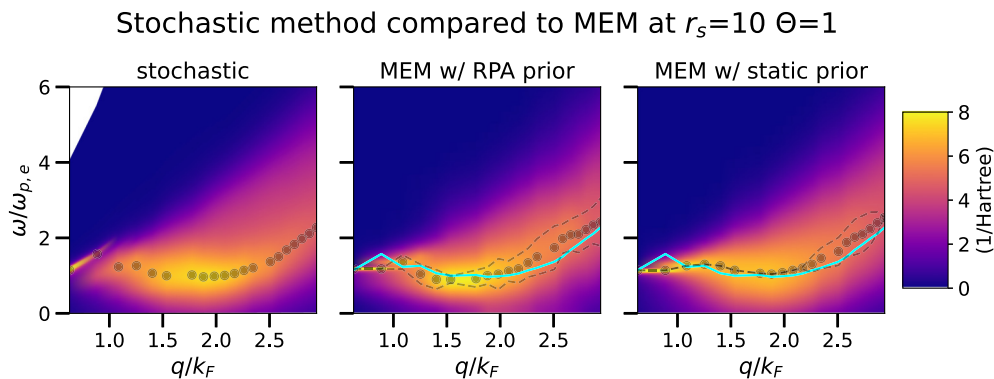


FIG. 2. Heat maps of the DSF $S(q, \omega)$, which compare our MEM inversions to the results of Dornheim *et al.* [27], which were computed with a stochastic algorithm [28]. For each q , black dots are placed at the maximum value of the DSF. Together these curves indicate the dispersion relation. Dashed black lines indicate twice the standard deviation of the location of the DSF maximum across leave-one-out bins. For comparison, we include the stochastic DSF peak location as a solid cyan line.

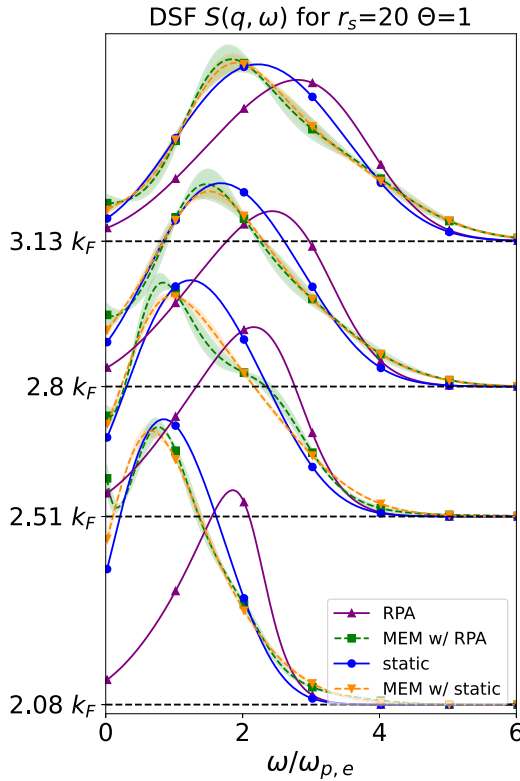


FIG. 3. Stacked q cross sections for $S(q, \omega)$, ω is varied along the x -axis, and dashed black lines indicate the zero position for each corresponding q cross section. The plot titles indicate the corresponding r_s and Θ values. The shaded dark orange and green regions indicate the error of the MEM estimate computed via (9).

Both SHAN and 9MA manifest a redshift in the roton feature compared to the static approximation, a result with which we agree. The biggest difference between the results is that the 9MA approach manifests a second peak in the DSF, deemed a double plasmon excitation, while the SHAN approach does not. In Fig. 3, we plot our DSF estimates for $r_s = 20$, which corresponds to the region where the 9MA observed the double plasmon excitation. However, our results have no second peak. On the contrary, we see that the MEM w/ RPA prior reduces the RPA peak in that region, and the MEM w/ static prior does not introduce a second bump in that region. Thus, the fidelity term is not encouraging a double plasmon excitation for $r_s = 20$. Instead, we find evidence for an incipient double peak at $r_s = 200$, as will be demonstrated later in Fig. 5. In short, we find very good agreement with their SHAN method.

We also agree with Fillinov *et al.*'s use of the goodness-of-fit criteria,

$$\delta F_r(q) = \frac{\Delta\tau}{\beta} \sum_i^{N\tau} \frac{\delta F(q, \tau_i)}{F^{\text{QMC}}(q, \tau_i)}. \quad (10)$$

For an analytic continuation estimate, $\delta F(q, \tau_i)$ is the absolute deviation between the data and the Laplace transformed estimate, i.e., $\delta F(q, \tau_i) = |F(q, \tau_i) - F^{\text{QMC}}(q, \tau_i)|$. For the data, $\delta F(q, \tau_i)$ is the statistical uncertainty. Equation (10) is essentially a discrete mean value theorem, indicating the average relative deviation from the data mean.

Using the goodness-of-fit criteria (10), the MEM estimates given in Fig. 3 score as follows: $q = 2.08k_F$ scores $\delta F_r(q) = 1.2 \times 10^{-3}$, $q = 2.51k_F$ scores $\delta F_r(q) = 2.0 \times 10^{-3}$, $q = 2.8k_F$ scores $\delta F_r(q) = 1.4 \times 10^{-3}$, and $q = 3.13k_F$ scores $\delta F_r(q) = 2.3 \times 10^{-3}$. Further, our data score as ≈ 0.04 for all q . For comparison, at $\Theta = 1$, across r_s and q , the 9MA typically scores $O[10^{-2}]$, the SHAN typically scores $O[10^{-1}]$, and the data itself typically score around 0.2. Based on Filinov *et al.*'s metric, we draw two conclusions. First, our data have an order of magnitude less statistical uncertainty, and second, our MEM estimates provide an order of magnitude better agreement with these more precise data.

C. Presentation of dynamic structure factor estimates at large coupling

Our ability to estimate the DSF at large r_s depends on our use of the static approximation as the Bayesian prior. Thus, we first compare our MEM DSF estimates with either RPA and static LFC priors for r_s values $r_s = 50, 100, 200$, which corresponds to a coupling parameter $\Gamma = 38.4, 76.8, 154$. Heatmaps of the Bayesian priors and the associated MEM results are given in Fig. 4. We see that using the RPA as a Bayesian prior produces significantly worse results for large r_s . In other words, the heatmaps depict volatile dispersion relations and multipeak structures. Additionally, heatmaps of the uncertainty are given in Fig. 11 located in Appendix B, and these heatmaps show that using the RPA as the Bayesian prior leads to larger relative uncertainty.

We expect that using the RPA as the Bayesian prior will lead to a horrible performance at strong coupling $\Gamma \gg 1$, because the assumptions of the RPA no longer apply. Comparatively, better performance is expected for the static approximation, whose assumptions are not violated by large r_s . Practically, the RPA Bayesian prior leads to volatile results because of the very narrow peak that is unaware of the roton feature. In solution space, such a Bayesian prior puts the minimum of the entropic term far away from the minimum of the fidelity term, so that small changes to the regularization weight can drastically change the solution. In short, using the broader static LFC as the Bayesian prior leads to more stable behavior.

Examining the behavior of the DSFs in Fig. 4, DSFs obtained with either prior exhibit a roton feature. The existence of the roton feature can be understood via the pair alignment argument discussed in Sec. II B 1 and originally proposed in Ref. [42]. In the case of the RPA as the Bayesian prior, the roton feature is created completely by the fidelity term in (2), since RPA neglects this. Thus, we take the MEM w/ RPA prior heatmaps as evidence that the roton feature is a genuine feature of the data. In the case of the static LFC as the Bayesian prior, the fidelity term redshifts the roton feature (see Fig. 5). This matches the typical relation between dynamic local field corrections and static local field corrections [30,42,91]. We take this as evidence that the MEM fidelity term is including the dynamic exchange-correlation effects, contained in the ITCF, into the DSF estimate. Lastly, for $r_s = 200$ there appears, spuriously, to be a strong excitation at zero frequency because the roton feature is redshifted towards zero. This is just a feature of the plotting; the DSF peak

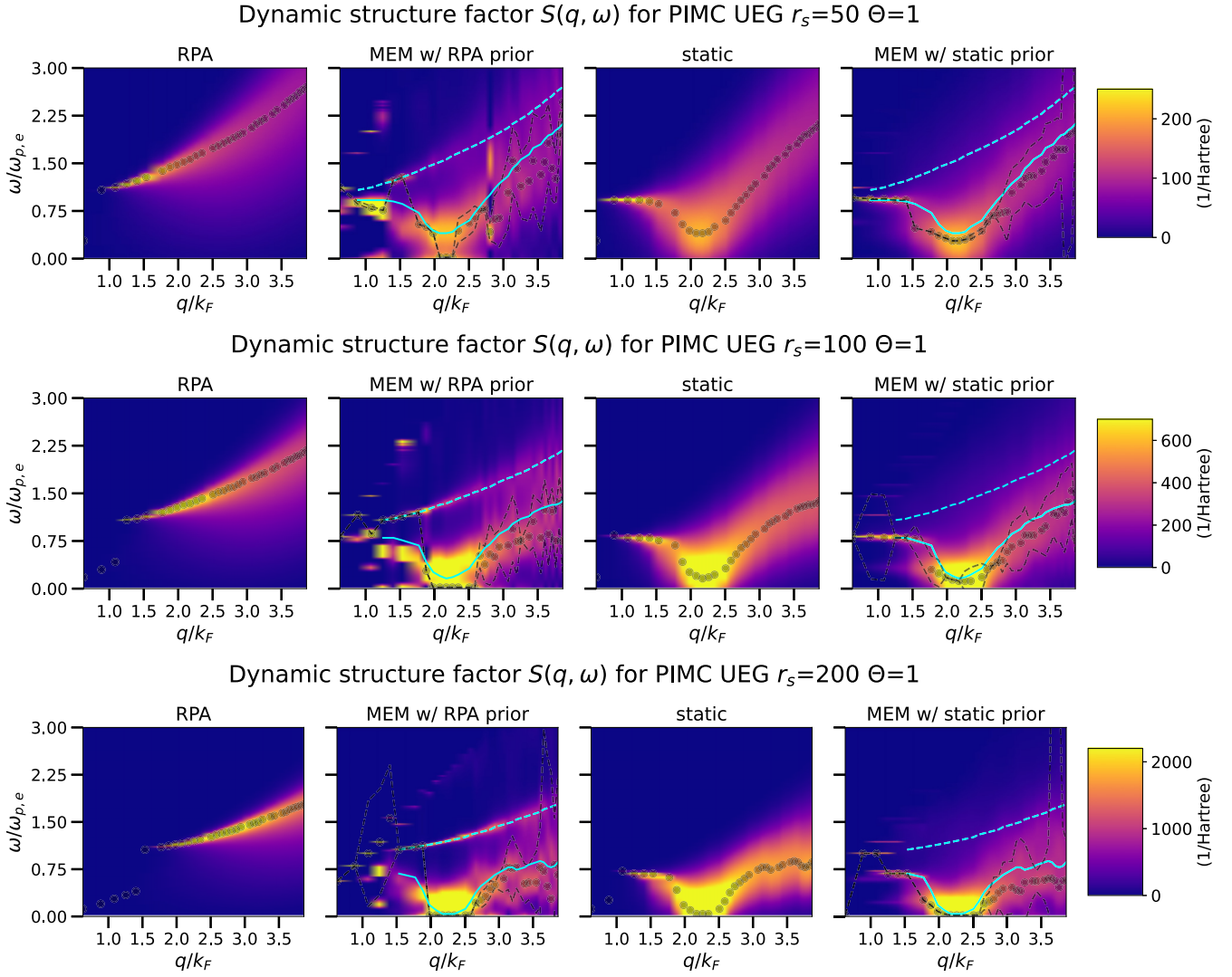


FIG. 4. Heat maps of $S(q, \omega)$ at quantum degeneracy parameter $\Theta = 1$ and Wigner-Seitz radius $r_s = 50, 100, 200$. The first column from the left contains the RPA DSF given by (4) and (5) with $G(q, \omega) = 0$. The second column contains the MEM estimate of the DSF using the RPA DSF as the Bayesian prior. The third column contains static LFC DSF, given by (4) and (5) with $G(q, \omega) = G(q, \omega = 0)$. The fourth column contains the MEM estimate of the DSF using the static DSF as the Bayesian prior. For each q , black dots are placed at the maximum value of the DSF. Together these curves indicate the dispersion relation. Dashed black lines indicate twice the standard deviation of the location of the DSF maximum across leave-one-out bins. For comparison, we include the RPA DSF peak location as a dashed cyan line and the static approximation DSF peak as a solid cyan line.

location is not at our smallest ω value. Again examining the DSFs in Fig. 4, we find that outside the $q \rightarrow 0$ limit, the MEM DSF estimates have their largest values at intermediate wave numbers $2 < q/k_F < 2.5$. This is a qualitative disagreement with the RPA model, which has a peak height that only reduces with q and a peak width that only broadens. This same qualitative disagreement persists in the $\omega \rightarrow 0$ limit. As we will see in Sec. III E, Fig. 8, the system's response to a static perturbation $\chi(q, \omega = 0)$ has a sharper peak than the RPA in this region. This qualitative disagreement grows with coupling, indicating that the exclusion of exchange correlation effects is the root cause. Fixed q cross sections from these heatmaps have been plotted in Appendix D. They show, for the interested reader, how the DSF peak narrows, increases in height, and shifts to lower ω values. Next, we examine

the $q = 2.8729k_F$ cross section from the heatmaps in Fig. 4. While the priors differ substantially, the final MEM results differ less than the underlying priors. At $r_s = 50$ the results are in general agreement, but the error associated with the static prior is smaller than the RPA prior. The agreement deteriorates because the MEM w/ RPA prior manifests an increasingly prominent second peak with increasing r_s . Since the second peak becomes more pronounced as the RPA becomes more peaked, i.e., a more restrictive prior, we do not take this as strong evidence of a double peak structure. However, for $r_s = 200$, the MEM w/ static prior exhibits an inflection point near the RPA peak location. We take this as stronger evidence of a double peak structure because the static approximation has no such peak near the RPA peak. This incipient double peak is similar to what has also been observed in classical

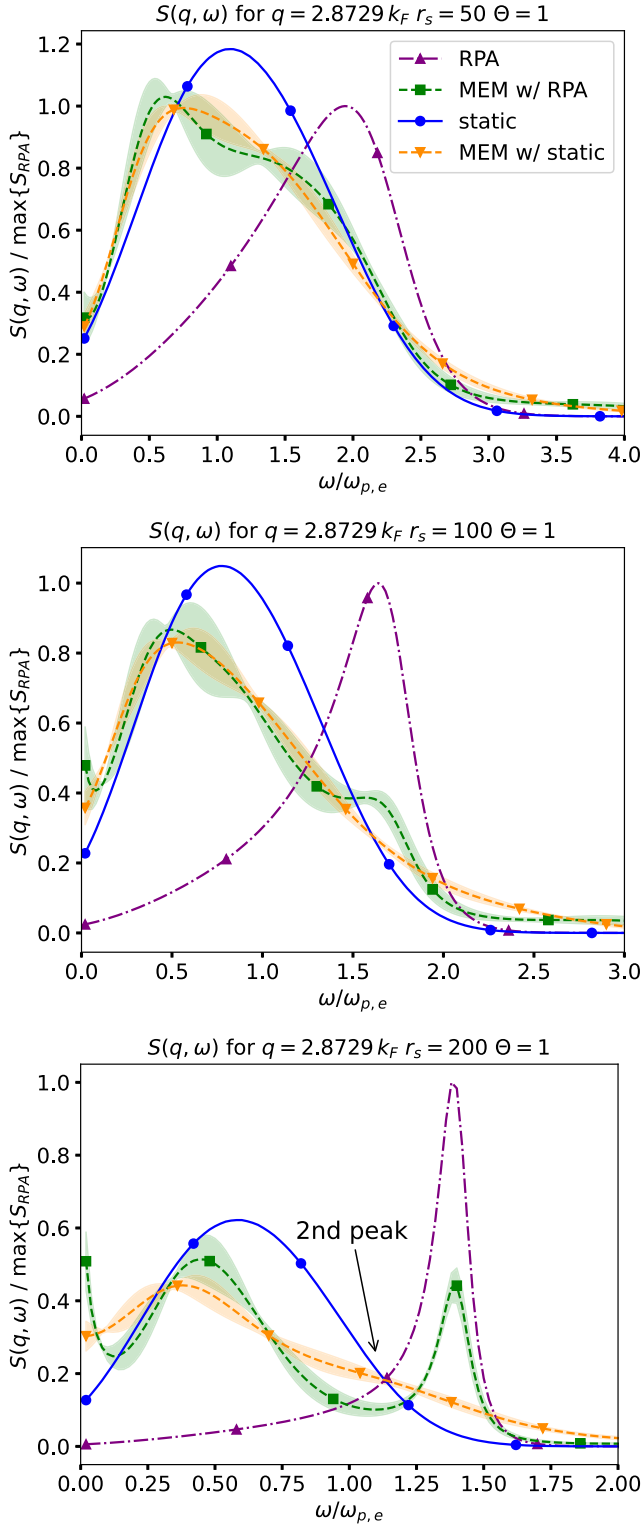


FIG. 5. Plots of $S(q, \omega)$ at $q = 2.8729 k_F$ for Wigner-Seitz radius $r_s = 50, 100, 200$. The legend in $r_s = 50$ indicates which colors/symbols correspond to MEM estimate and its associated Bayesian prior. For $r_s \geq 100$, the RPA becomes sufficiently narrow that the entropic regularization forces a peak into the estimate in the domain $[\omega_{p,e}, 2\omega_{p,e}]$. Comparatively, at $r_s = 200$, the static approximation, which has no peak in that domain, produces an inflection point marked “2nd peak.”

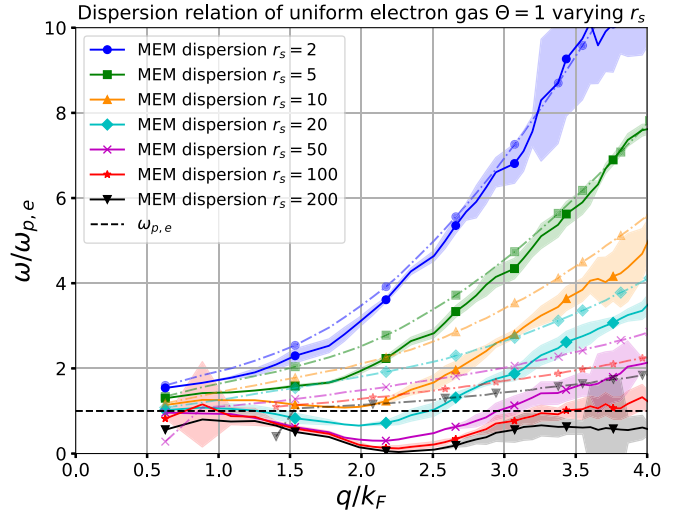


FIG. 6. Plot of the dispersion relation for $S(q, \omega)$ with varying r_s . The solid lines indicate our estimate using MEM with the static LFC as the Bayesian prior. For comparison, we include the RPA's dispersion relation as dashed lines. We set each dispersion curve's color and symbol based on the corresponding r_s value. For small r_s (i.e., weak coupling), our MEM reconstructions agree with the RPA dispersion curve within the error (9). For large r_s , a clear roton-type feature emerges, which is substantiated by the narrow error bands.

one-component strongly coupled Coulomb systems (SCCS) [51,52] as well as in the UEG [30,44,53,94]. For both systems, the double peak is understood as a dynamic effect.

D. Presentation of dispersion relation estimates across all r_s

We plot dispersion relations for MEM w/ static prior across all $r_s = 2, 5, 10, 20, 50, 100, 200$ in Fig. 6, limiting ourselves to the MEM results using the static LFC prior; RPA dispersions (dash-dotted curves) are also shown for reference. To the authors' knowledge, this is the largest range of r_s values that have been computed and collected. Examining the behavior at large r_s , the MEM dispersion relation differs substantially from the RPA. In particular, the peak $\omega(q)$ of the dynamic structure factor $S(q, \omega)$ exhibits a nonmonotonic wave-number dependence with an inflection point q_I , such that $\partial_q \omega(q) < 0$ for $q < q_I$ and $\partial_q \omega(q) > 0$ for $q > q_I$. These curves establish that exchange-correlation effects grow with r_s , as expected. In total, this plot demonstrates on this q, ω domain a smooth continuation of known features into higher coupling.

E. Presentation of sum rules for dynamic structure factor estimates

A crucial assessment for a DSF is the fulfillment of relevant sum rules [52,109]. Each sum rule establishes whether certain physics is present in the DSF model. We consider the following sum rules:

$$\langle \omega^{-1} \rangle = -\frac{\chi(q, 0)}{2n} = \frac{1}{2} \int_0^\beta d\tau F(q, \tau), \quad (11)$$

$$\langle \omega^0 \rangle = S(q) = F(q, \tau = 0), \quad (12)$$

$$\langle \omega \rangle = E_F \left(\frac{q}{k_F} \right)^2 = -\frac{\partial}{\partial \tau} F(q, \tau) \Big|_{\tau=0}, \quad (13)$$

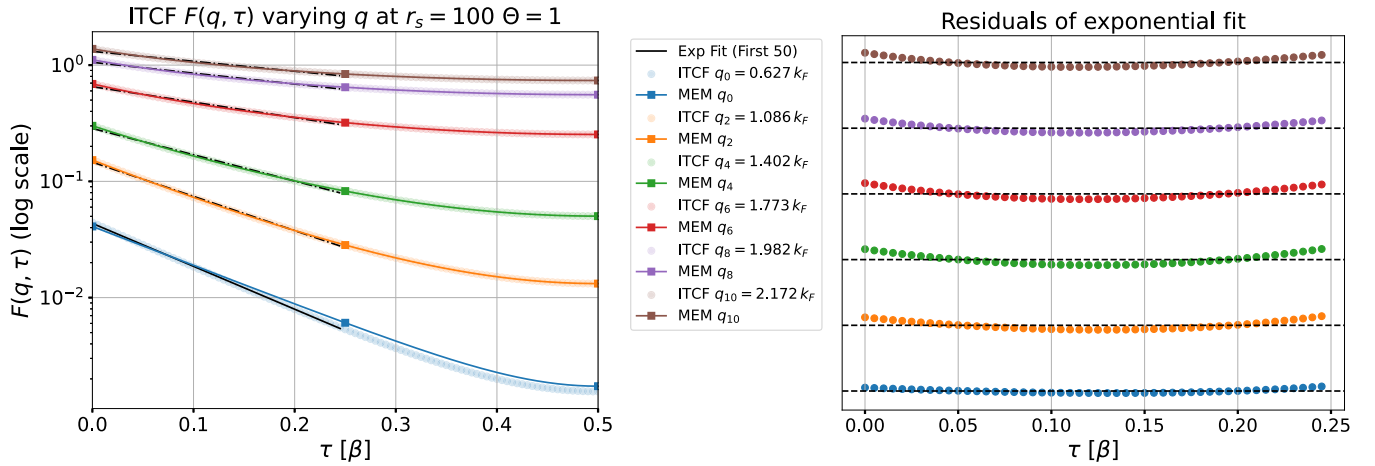


FIG. 7. The left plot is of the Laplace transform of the MEM DSF estimate compared with the ITCF data for $r_s = 100 \Theta = 1$ for the first half of the symmetric τ domain; these two curves are indistinguishable. We also include exponential fits on the first 50 data points of the ITCF. In the right plot, we show the residuals of the single exponential fit. As $q \rightarrow 0$, the systematic errors in the residuals vanish. This implies that the ITCF is best explained by a single Dirac δ function DSF and explains the integration convergence issues for large r_s at small q in Fig. 8.

where the average is defined $\langle \omega^k \rangle \equiv \int d\omega \omega^k S(q, \omega)$. The first equality in (11), presented in [89,110], tells us that the static density response function is sensitive to when the DSF's peak is located at small ω . So for systems with a roton feature, we expect larger density response to intermediate wave numbers q . The second equality, presented, e.g., in [89], tells us that if the integral of the ITCF is small, then there is little density response. This integral is strongly dependent on the decay rate of the ITCF, which by definition expresses the quantum delocalization in the system. Hence, quantum delocalization reduces density response. Equation (12) defines the static structure factor $S(q)$, which represents the average spatial correlations in the system [3,111]. Finally, Eq. (13) defines the F-sum rule, which tells us whether the continuity equation $\mathbf{k} \cdot (n_0 \delta \mathbf{u}) = \omega \delta n$ is satisfied [3,57,108].

As stated, the MEM is not guaranteed to satisfy any of the sum rules (11), (12), or (13). However, it is known that moments of the DSF can be related to the derivatives of the ITCF at $\tau = 0$ [92,112],

$$(-1)^n \left(\frac{\partial}{\partial \tau} \right)^n F(q, \tau) \Big|_{\tau=0} = \int_{-\infty}^{\infty} d\omega \omega^n S(q, \omega). \quad (14)$$

Consider (14) as a finite difference expression. Since there are no data for $\tau < 0$, estimating the n th derivative (and hence the n th moment) requires $n + 1$ points from $\tau = 0$. Further, consider a Taylor expansion of $F(q, \tau)$. To properly represent a function further from the Taylor expansion point $\tau = 0$ requires higher moments in the Taylor expansion. As such, the information on higher moments is contained away from $\tau = 0$, while the information for the lower moments is contained near $\tau = 0$. Thus, if the PIMC ITCF data satisfy the sum rules, this occurs because minimizing the generalized least squares criteria (2) (i.e., selecting a DSF that matches the data) implicitly enforces the correct sum rule behavior. From this perspective, satisfying known sum rules is a nontrivial test of our analytic continuation algorithm's ability to extract information from the data. Furthermore, higher power moments

are suppressed by a factor $1/n!$, so each successively higher moment is a more challenging test than the previous one.

For $r_s = 100$ and $\Theta = 1$, we visualize the agreement between the ITCF data and the Laplace transform of the DSF estimate; the Laplace transformed DSF is indistinguishable from the ITCF (see Fig. 7, left). Based on (14) as well as the discussion around this equation, the numerical agreement between the Laplace transform of the DSF and the ITCF indicates we should expect that the reconstruction will satisfy sum rules, even though the MEM criteria do not enforce them explicitly. We also include in Fig. 7 an exponential fit and residuals of the exponential fit. These residuals show that, as $q/k_F \rightarrow 0$, a single exponential fit does not have systematic bias, demonstrating that the DSF is converging to a Dirac δ . This is expected for $q \rightarrow 0$, where the DSF typically converges to a Dirac δ located at $\omega = \omega_{p,e} \delta(\omega - \omega_{p,e})$ [76,108].

Let us next investigate the performance of the MEM solutions with respect to the sum rules, Eqs. (11)–(13). First, we investigate the static structure factor (12). Plots are given in Fig. 8, left. These plots demonstrate that our MEM results closely follow the static approximation but match the PIMC data $F(\tau = 0)$ better for large r_s . Overall, the MEM estimates have a smoother convergence to $S(q) = 1$ in the $q \rightarrow \infty$ limit and to $S(q) = \frac{\hbar^2 q^2}{2m_e} (\hbar \omega_{p,e})^{-1} \coth(\beta \hbar \omega_{p,e}/2)$ in the $q \rightarrow 0$ limit than either Bayesian prior. We remind the reader that, for large r_s , in the $q \rightarrow 0$ limit, the DSF is converging to a Dirac δ , and numerical integration fails. This leads to false zeros for the static and RPA $S(q)$.

We also investigate the frequency sum rule (F-sum rule) (13) in Fig. 8, middle. These plots demonstrate that our MEM results numerically satisfy the F-sum rule for all q values. Based on (14), this tells us that the Laplace transform of our DSF estimates has a first derivative that closely matches the first derivative of the ITCF data near $\tau = 0$ and that the DSF is converging to a Dirac δ in the small- q limit.

Finally, we investigate the MEM estimate's inverse moment sum rule (11) in Fig. 8, right, which is sensitive to when the DSF peak is located at small ω . We find good

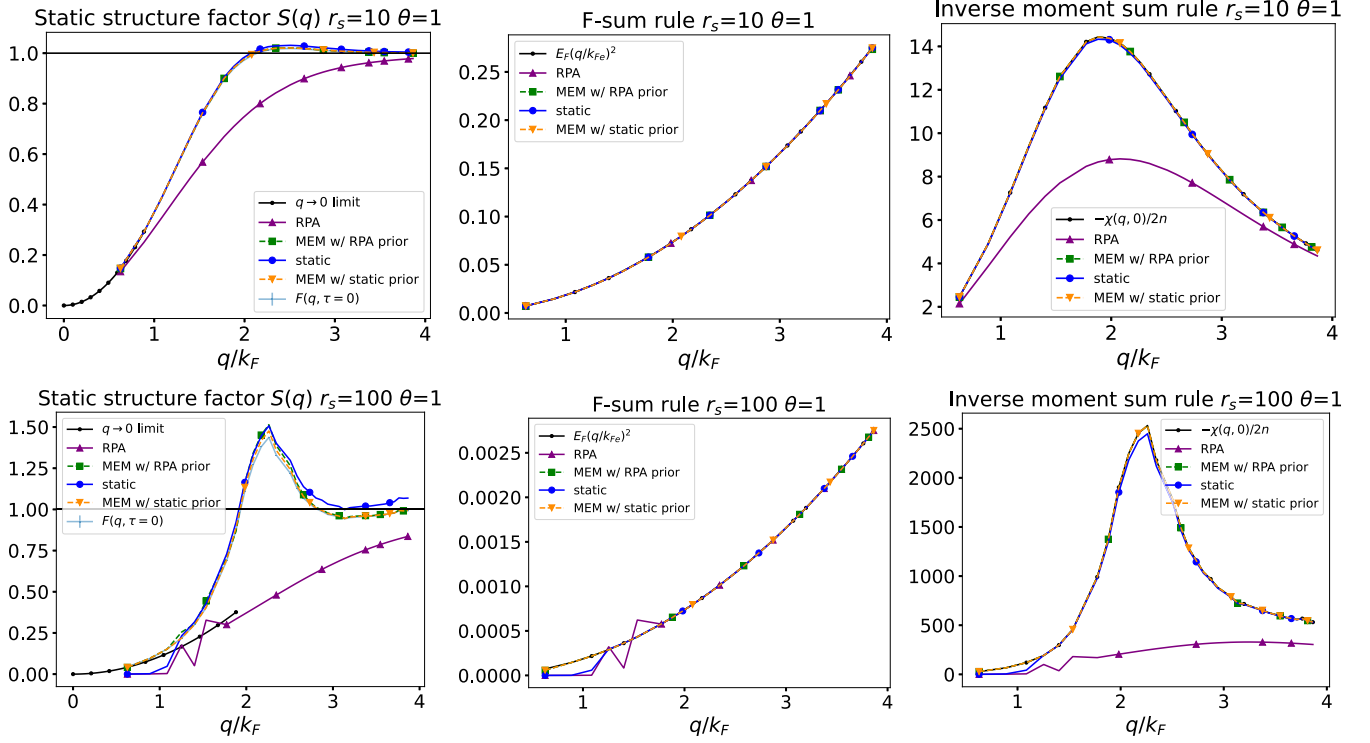


FIG. 8. We plot the inverse moment sum rule (11), the static structure factor (12), and the F-sum rule (13) for $r_s = 10$ and 100. For large r_s , the DSF peak is so narrow in the $q \rightarrow 0$ limit that numerical integration fails; this is already discussed in Fig. 7. Further, for large r_s , slight deviations exist between the inverse moment sum rule $-\chi(q, 0)/2n$ and the static LFC DSF, but not the MEM estimates; this is discussed in Appendix A.

numeric agreement across all $r_s = 2, 5, 10, 20, 50, 100, 200$ values. See Appendix E for other r_s values. Comparatively, the static approximation has a slight deviation from this sum rule for $r_s = 100$ between $q = 2k_F$ and $2.5k_F$. Although this slight deviation is hard to notice, it is still worth mentioning because the static LFC is guaranteed to satisfy the inverse moment sum rule; see Appendix A. This feature may arise when computing the DSF via (5) at a given r_s and θ , because there is a small inconsistency. The static LFC $G(q, \omega)$ is being calculated from PIMC simulations with finite N particles, while the ideal-susceptibility $\chi^0(q, \omega)$ is being calculated assuming the thermodynamic limit, i.e., $N \rightarrow \infty$ particles. However, we found that doubling the number of particles did not reduce the magnitude of this discrepancy; see Fig. 10. Therefore, the origin of this issue is unknown. In Appendix A, we also discuss why the MEM estimates, which are not guaranteed to satisfy the inverse moment sum rule, perform better than the static approximation.

IV. SUMMARY AND CONCLUSIONS

In this work, we have estimated DSFs of the finite temperature electron liquid from PIMC ITCF data (see Table I) by direct inversion of the two-sided Laplace transform using the MEM. We constructed the MEM's Bayesian prior via (4) and (5) after computing the static LFC $G(q, \omega = 0)$ from our data. We conducted the MEM within a leave-one-out resampling routine, which provided appropriate error quantification (9);

see the error bands on the dispersion relations in Fig. 6 and heatmaps of relative error in Fig. 11 of Appendix B.

We have considered the physics and data science of constructing the static LFC from the data to be used as the MEM's Bayesian prior. Investigations have shown that the static approximation gives a reasonable description of the dispersion relation, but it fails to capture all of the collisional damping in a plasma. As such, using the static LFC $G(q, \omega = 0)$ means we are focusing the MEM on extracting the frequency dependence of $G(q, \omega)$. In particular, at large r_s values, the RPA does not even qualitatively describe the DSF, and using the RPA as the Bayesian prior produces low quality results. By comparison, the static LFC Bayesian prior remains valid and the MEM results are stable (see Fig. 4). We discuss from the data science perspective that computing $G(q, \omega = 0)$ from the data is informing the MEM of the ITCF's average value (6). This resembles typical detrending approaches in data science, focusing the MEM's inference abilities on deviations from the mean. Further, from the statistics perspective, using an entropic regularization with a Bayesian prior estimated from the data mitigates the bias introduced by regularization.

We have shown that our DSFs recover the RPA form at small r_s and $\Theta = 1$; see Fig. 1. Further, our DSF estimates resemble preexisting calculations of the DSF at moderate r_s values, but they score orders of magnitude better on goodness-of-fit metrics; see Figs. 2 and 3. In particular, when the MEM uses the static approximation as a Bayesian prior, it produces a DSF estimate that differs from the static approximation in ways that are similar to how dynamic local field correction

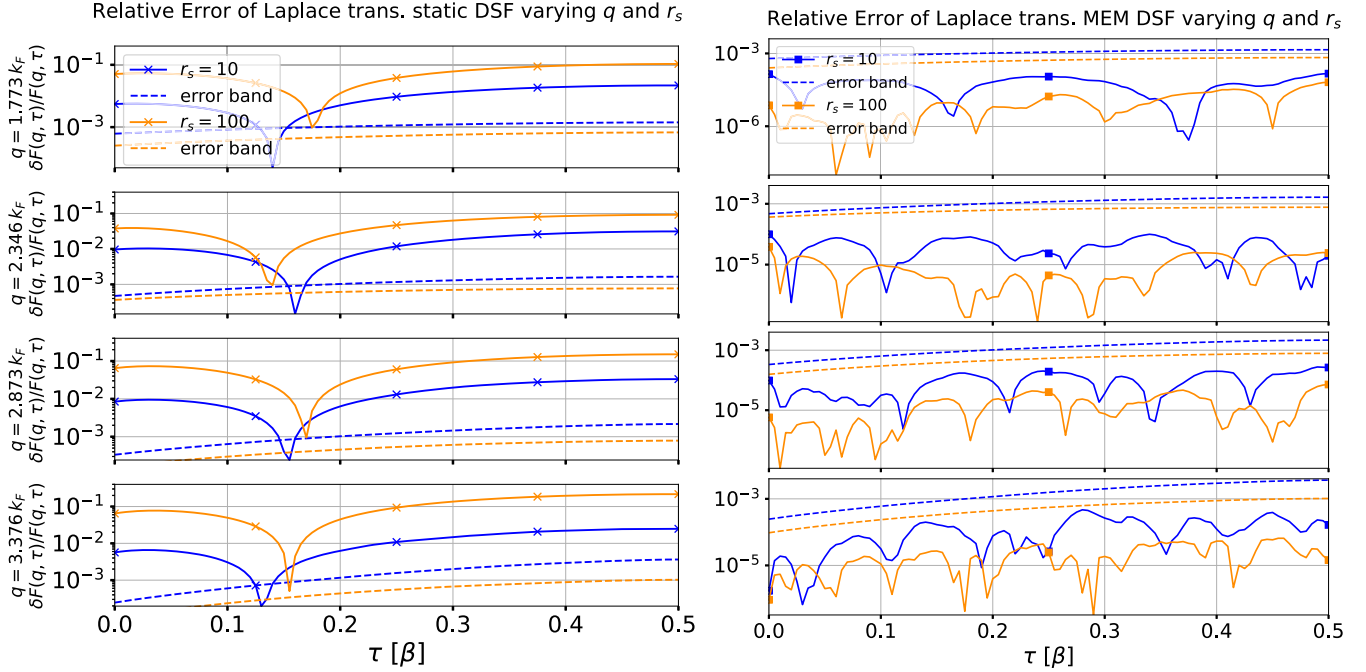


FIG. 9. Plot of the relative residuals from the ITCF data for the static approximation DSF (left) and the MEM w/ static prior DSF (right) for the first half of the symmetric τ domain. Notice, the y-axes are not the same for the left and right plots, but the relative error (error band) is shared on both plots to help recognize the order of magnitude difference. The residuals associated with the static approximation have a unique systematic trend, where the magnitude of this systematic trend varies with both r_s and q . Comparatively, the residuals associated with the MEM are orders of magnitude smaller and appear as oscillations with no definitive q and r_s dependence.

approaches differ from the static approximation. We take this as evidence that the MEM is using the data to incorporate the dynamic dependency of the local field correction.

In Sec. III E we have checked that our DSFs satisfy the large- and small- q limits for the static structure factor, the F-sum rule, and the ω^{-1} sum rule (see Fig. 8). Satisfying these sum rules is significant because the MEM does not enforce them as solution constraints. Since the sum rules are contained in the derivatives of the ITCF data, whether

or not they manifest in the MEM estimates is determined solely by the goodness of fit (i.e., least squares criteria). The quality of the fits is visualized in Fig. 7. We also assess our $r_s = 20$ fits by the average relative residual (10) in Sec. III B 3 and visualize the relative residuals across τ for $r_s = 100$ in Fig. 9.

The present study covers the regime of substantially lower density and, hence, stronger coupling compared to previous investigations [27,30]. Our investigations have established new results at strong coupling. Using the static LFC as our Bayesian prior, the MEM produces DSFs which contain a roton feature for $r_s \gtrsim 10$ (see Fig. 6). Our DSFs show a more pronounced roton feature than the static LFC (see Figs. 4, 12, and 13), as is expected. Moreover, the redshift in the roton feature increases smoothly with r_s into stronger couplings (see Fig. 6), as is predicted by the recent semiempirical pair alignment model [42]. Finally, we find at $r_s = 200$ that the MEM estimates exhibit an incipient double peak structure (see Fig. 5). We do not find evidence for a double peak structure at $r_s = 20$, disagreeing with Filinov *et al.*'s 9MA estimates, but agreeing with their SHAN estimates [30]. Investigating this, we found that according to Filinov *et al.*'s own goodness-of-fit metric, we have better data and our MEM estimates better fit our better data.

Future work can apply these DSF estimates to the applications discussed in the Introduction: establishing frequency-dependent exchange-correlation kernels for TD-DFT, computing dielectric functions and transport properties for kinetic or hydrodynamic simulations, using UEG DSFs as input for the interpretation of x-ray Thomson scattering experiments

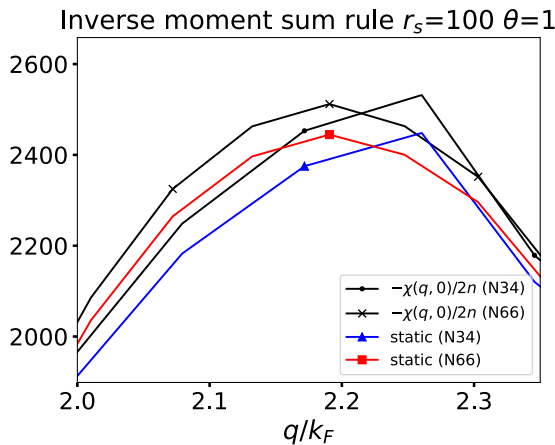


FIG. 10. Plot of the inverse sum rule for the static approximation at $r_s = 100$ and two different numbers of particles, indicated by the legend. The plot is zoomed-in on the peak region where the discrepancy exists and persists at higher number N .

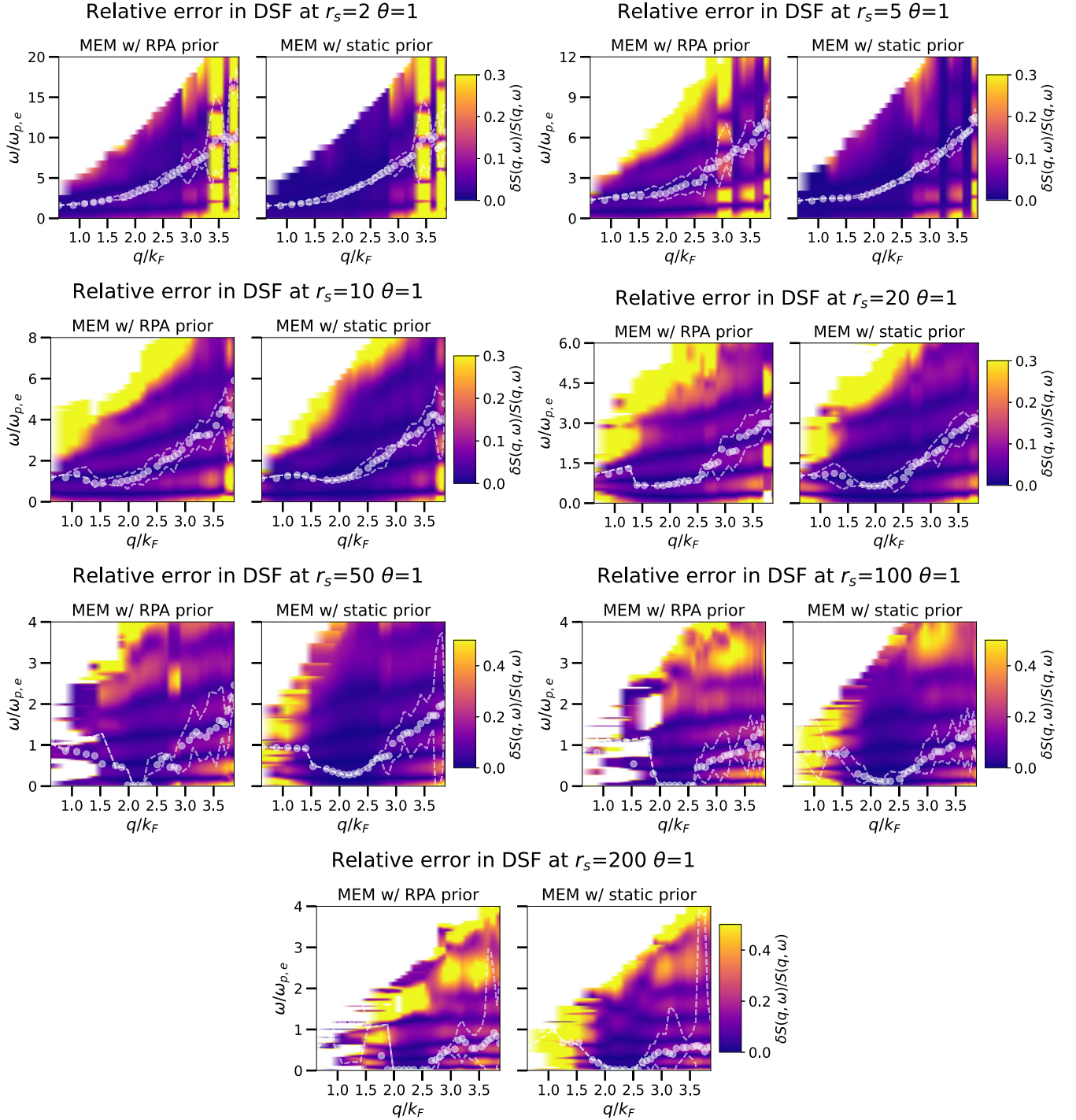


FIG. 11. Heat maps of the relative error in the MEM estimate $\delta S(q, \omega)/S(q, \omega)$. Plot titles indicate the corresponding r_s and Θ values, as well as which Bayesian prior was used. Error $\delta S(q, \omega)$ is quantified using (9). As $S(q, \omega) \rightarrow 0$ goes to zero $\delta S(q, \omega)/S(q, \omega)$ becomes unstable. Thus, for visual clarity we do not plot results where $S(q, \omega) < 10^{-3}$; this manifests as a white region. Using the RPA model results in a breakdown of the MEM estimate at small q . For each q , white dots are placed at the maximum value of the DSF. Together these curves indicate the dispersion relation. Dashed white lines indicate twice the standard deviation of the location of the DSF maximum across leave-one-out bins.

within the Chihara decomposition, and benchmarking new dynamic theories in the strongly coupled regime. Future work on the UEG can explore different default models and simulation parameters; the latter would be particularly helpful to inform new analytical or neural network representations of

the full dynamic local field correction in the real-frequency domain. Finally, we stress that the present MEM setup is not limited to the UEG and can be used to compute the electronic DSF of real warm dense matter systems such as hydrogen and beryllium, for which accurate PIMC calculations of the

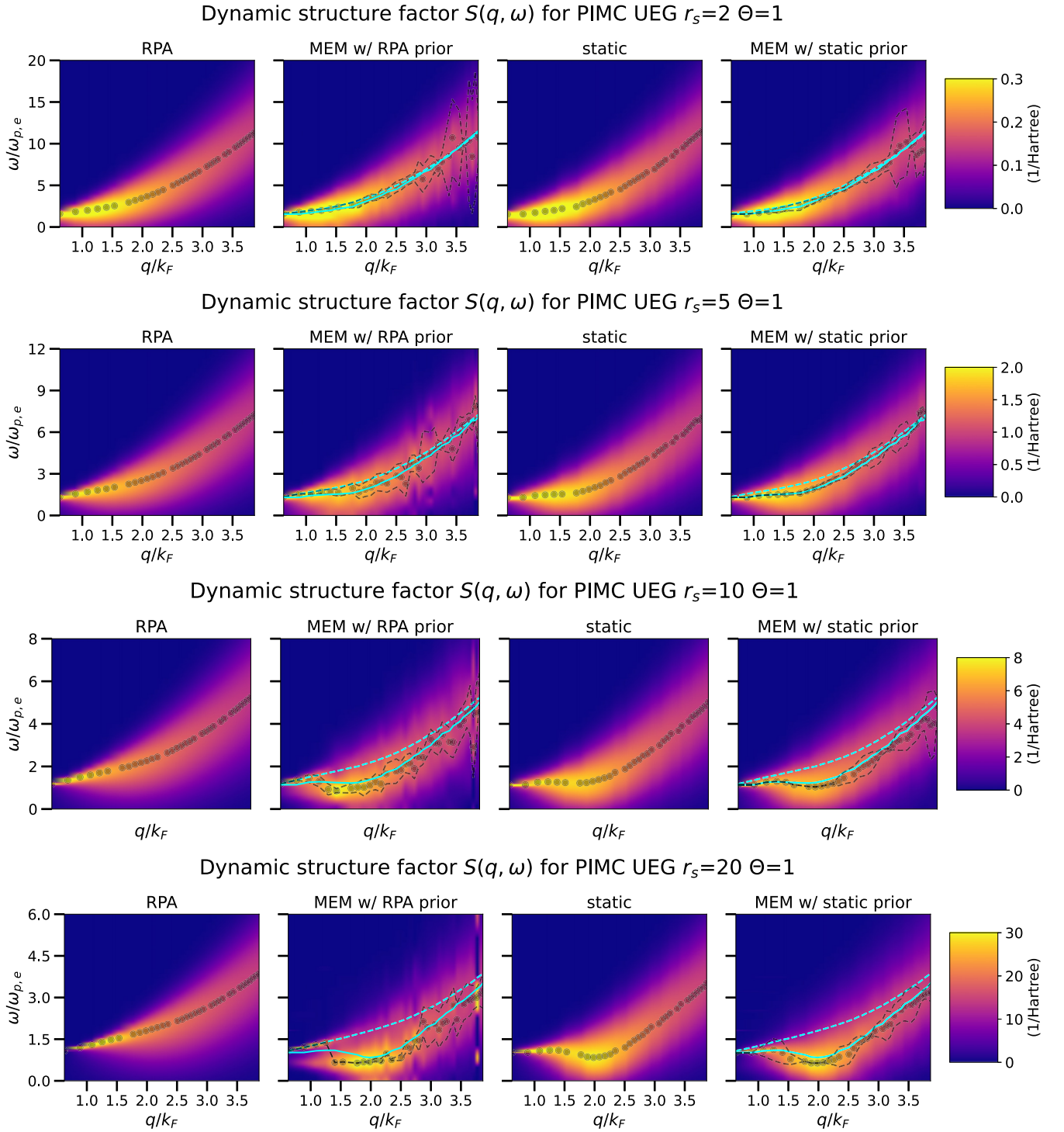


FIG. 12. Heat maps of $S(q, \omega)$ at quantum degeneracy parameter $\Theta = 1$ and Wigner-Seitz radius $r_s = 2, 5, 10, 20$. The first column from the left contains the RPA DSF given by (4) and (5) with $G(q, \omega) = 0$. The second column contains the MEM estimate of the DSF using the RPA DSF as the Bayesian prior. The third column contains static LFC DSF, given by (4) and (5) with $G(q, \omega) = G(q, \omega = 0)$. The fourth column contains the MEM estimate of the DSF using the static DSF as the Bayesian prior. For each q , black dots are placed at the maximum value of the DSF. Together these curves indicate the dispersion relation. Dashed black lines indicate twice the standard deviation of the location of the DSF maximum across leave-one-out bins.

ITCF have already been demonstrated [113–115]. This will allow for the PIMC informed prediction of x-ray Thomson scattering measurements, e.g., at the National Ignition Facility [116] or at the European XFEL [117], for the development of

improved model descriptions for the electronic dynamics of warm dense matter, e.g., within the Chihara decomposition [118], and to rigorously assess the accuracy of different time-dependent DFT methodologies [82, 119–122].

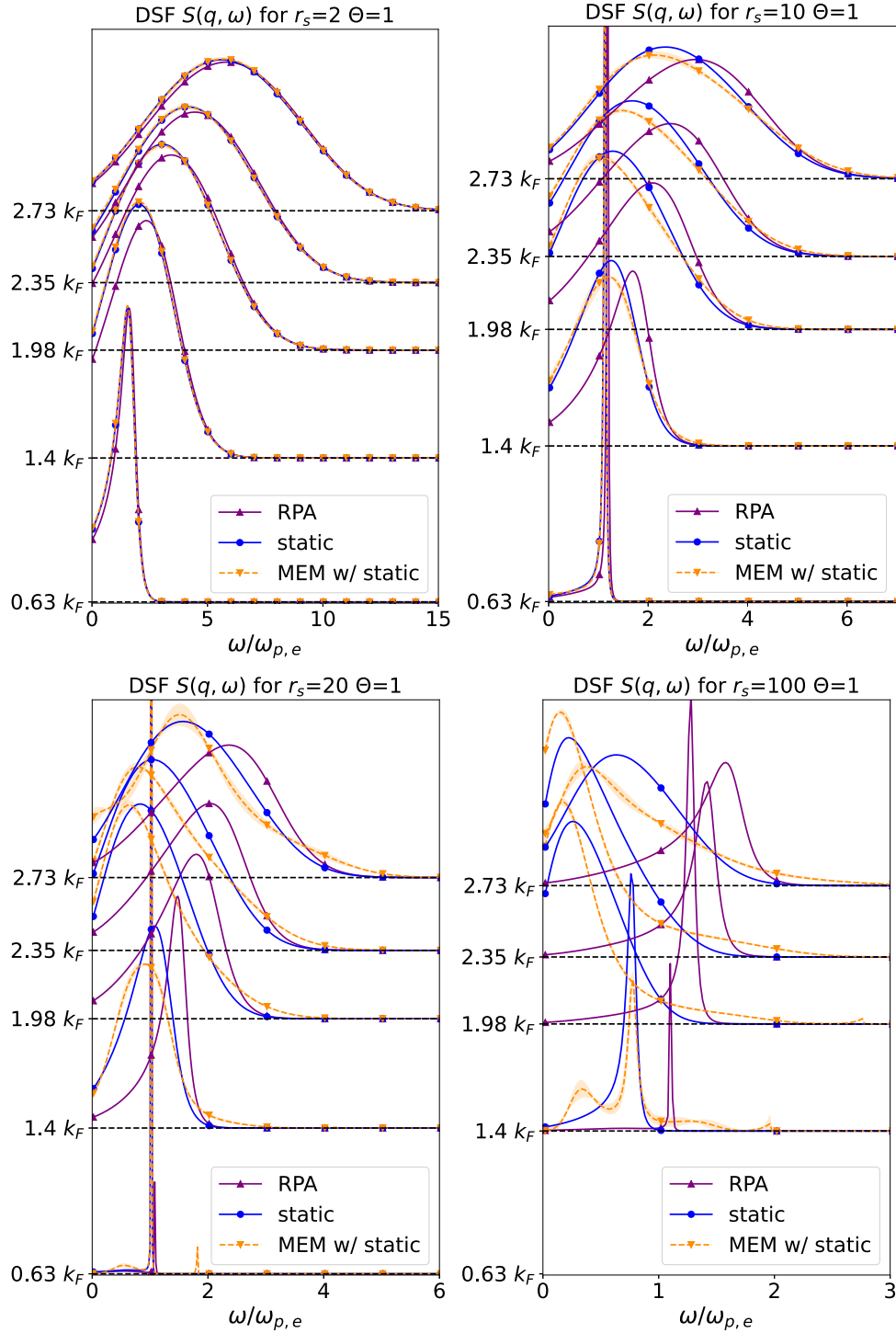


FIG. 13. Stacked q cross sections for $S(q, \omega)$. ω is varied along the x -axis, and dashed black lines indicate the zero position for each corresponding q cross section. The plot titles indicate the corresponding r_s and Θ values. The shaded dark orange regions indicate the error of the MEM estimate computed via (9). We neglect the $q = 0.63k_F$ curves in the right plot ($r_s = 100$, $\Theta = 1$) because the plasmon peak is too narrow to be resolved at our ω discretization. Relative to the RPA DSF (RPA) and static local field correction DSF (static), the MEM's estimate of the DSF (MEM w/ static) tends to reduce the width of the DSF and redshift the peak.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [107].

APPENDIX A: INVERSE MOMENT SUM RULE

In this Appendix, we establish that the static local field correction satisfies the inverse moment sum rule. For the reader's convenience, we repeat the inverse moment sum rule (11),

$$\langle \omega^{-1} \rangle = \int_{-\infty}^{+\infty} \frac{1}{\omega} S(q, \omega) = \frac{1}{2} \int_0^\beta d\tau F(q, \tau). \quad (\text{A1})$$

Inserting the definition of the DSF (5) and simplifying, we find

$$\langle \omega^{-1} \rangle = -\frac{1}{2\pi n} \int_{-\infty}^{+\infty} d\omega \frac{1}{\omega} \text{Im}\chi(q, \omega). \quad (\text{A2})$$

The Kramers-Kronig relations inform us that

$$\frac{1}{2\pi n} \int_{-\infty}^{+\infty} \frac{1}{\omega} \text{Im}\chi(q, \omega) = \frac{1}{2n} \text{Re}\chi(q, 0), \quad (\text{A3})$$

which has two consequences: first, it holds that

$$\langle \omega^{-1} \rangle = -\frac{1}{2n} \text{Re}\chi(q, 0), \quad (\text{A4})$$

which establishes the inverse moment sum rule; second, we have

$$\int_{-\infty}^{+\infty} \frac{1}{\omega} S^{\text{SLFC}}(q, \omega) = \frac{1}{2n} \text{Re}\chi^{\text{SLFC}}(q, 0), \quad (\text{A5})$$

but we also have by definition $\text{Re}\chi^{\text{SLFC}}(q, 0) = \text{Re}\chi(q, 0)$. Thus, S^{SLFC} satisfies the inverse sum rule. Notice that this derivation works for the inverse moment because we have Kramers-Kronig relations, and it does not work for positive moments $\omega^1, \omega^2, \dots$, where Kramers-Kronig relations cannot be invoked.

It is important to consider that the MEM, which is not guaranteed to satisfy this sum rule, does a better job than the static model for which the sum rule is, in theory, guaranteed. To understand this, consider (A1), which informs us that the inverse moment sum rule is essentially a check of whether the Laplace transformed DSF model $F^{\text{Model}}(\tau) = \int d\omega e^{-\tau\omega} S^{\text{Model}}(\omega, q)$ and PIMC ITCF $F(\tau)$ integrate to the same value. Hence,

a breakdown in the sum rule is a statement about the discrepancies between $F^{\text{Model}}(\tau)$ and $F(\tau)$. We investigate these discrepancies in Fig. 9. First, we see that such discrepancies exist in all the models plotted in Fig. 8. However, these discrepancies are much smaller for the MEM estimates because the fidelity term in the MEM regularization minimizes the $F^{\text{Model}}(\tau)$ deviation from $F(\tau)$. Thus, the fidelity term is automatically enforcing the sum rules, but only up to some numerical degree and not exactly. Also note that while the differences in the ITCF between the static approximation and the PIMC reference data for $r_s = 100$ are substantial, they are largely averaged out by the integration over τ . It is only the small residual of the τ -integral that violates the inverse moment sum rule, and this violation persists with increasing numbers of particles (see Fig. 10); the cause is currently unknown.

We demonstrate that doubling the number of particles does not improve the static approximation's inverse sum rule agreement with the static density response's peak in Fig. 10; the cause is currently unknown. This question might be resolved based on dedicated large-scale PIMC simulations of the electron liquid, which will be pursued in future works.

APPENDIX B: DSF ERROR ESTIMATES

In this Appendix, we present our uncertainty quantification across all r_s , q , and ω . Figure 11 contains heatmaps of the relative error $\delta S(q, \omega)/S(q, \omega)$, where δS is given (9). From these heatmaps, we see that using the RPA as a Bayesian prior produces DSF estimates that are less certain. Across all r_s , the uncertainty in the dispersion relation grows with q after the dispersion relation's inflection point. This arises because the DSF only populates large ω , making the ITCF decay quickly. Thus, at large q only a few points are not numerically zero, but more ω grid points need resolved. This results in greater uncertainty. We also observe a systematic ringing matching previous investigations of entropic regularizers [26]. By inspection, the solution does not contain this ringing. We take this as evidence that the Bayesian posterior is weighting the solutions appropriately.

Another feature of these heat maps is that as r_s grows, the uncertainty in small q grows. This occurs because, in this limit, the DSF is a very narrow Lorentz curve, converging to a Dirac δ function. This means that many DSF values are close to numerical zero, and any finite error yields a large relative error. For our application, convergence to a Dirac δ peak is desired, and we investigated this convergence in Sec. III E.

APPENDIX C: DSF HEATMAPS FOR $r_s \leq 20$

For completeness, we present heatmaps of the DSF for $r_s = 2, 5, 10, 20$ in Fig. 12. These are all r_s values outside the strong-coupling region. From these heatmaps, we see that the disagreement between MEM w/ RPA prior and MEM w/ static prior grows with r_s . Further, we see that the uncertainty band around the dispersion relation for MEM w/ RPA prior grows with increasing r_s . This reflects that the distance between the Shannon-Jaynes entropy minimum and the fidelity minimum are moving away from each other in solution space, increasing the solution's sensitivity to the

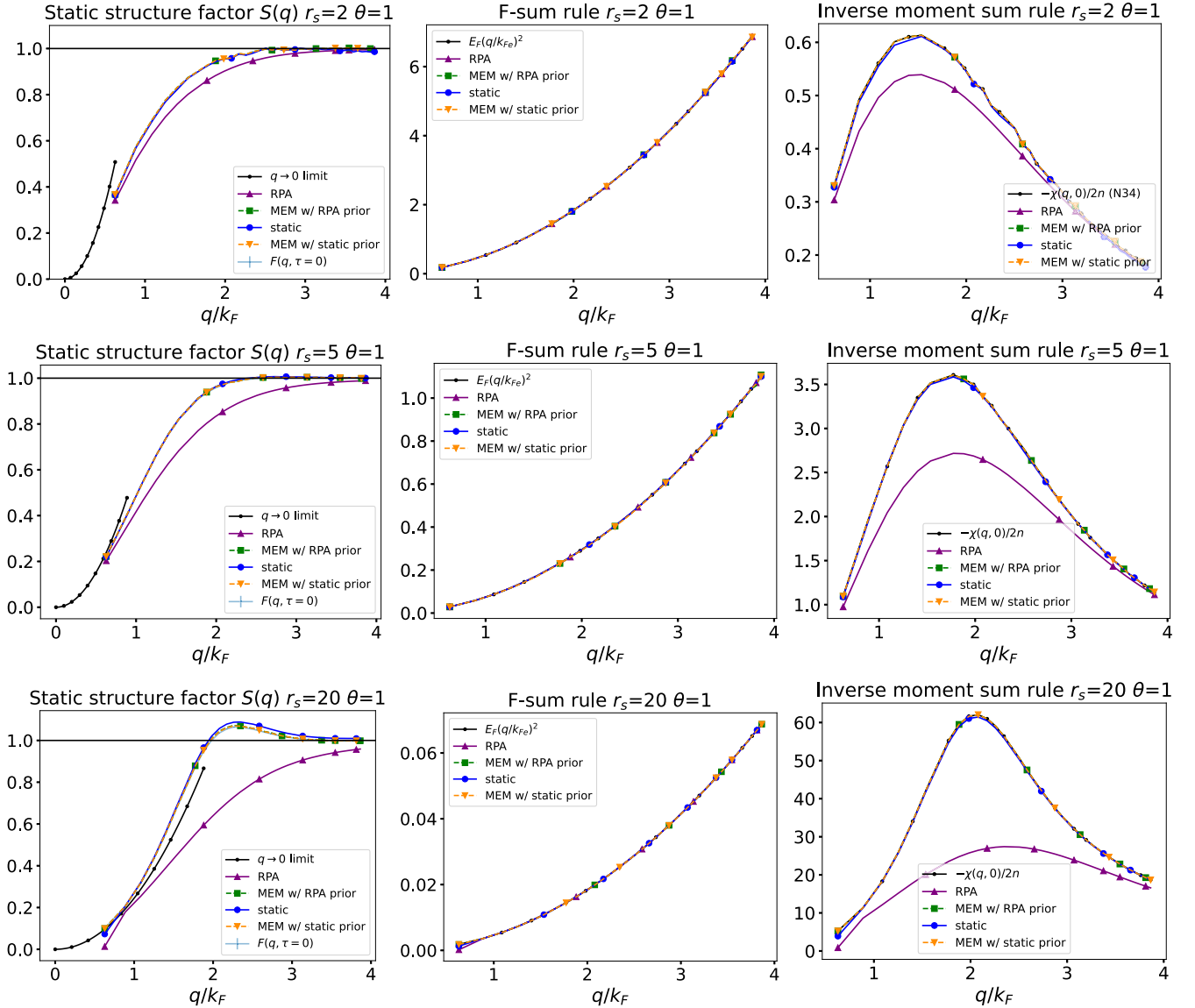


FIG. 14. We plot the inverse moment sum rule (11), the static structure factor (12), and the F-sum rule (13) for $r_s = 10$ and 100 . For large r_s , the DSF peak is so narrow in the $q \rightarrow 0$ limit that numerical integration fails; this was already discussed in Fig. 7. Further, for large r_s , slight deviations exist between the inverse moment sum rule $-\chi(q, 0)/2n$ and the static LFC DSF, but not the MEM estimates; this is discussed in Appendix A.

regularization weight. Lastly, these heatmaps do not have sharp or sudden changes with increasing r_s , which provides evidence that the roton feature grows smoothly with r_s .

APPENDIX D: DSF CROSS SECTIONS FOR SELECT r_s

In this Appendix, we provide DSF q cross sections in Fig. 13 and examine how the MEM estimates differ from the RPA and static approximation across q . We observe that these dynamic effects become more prominent than for $r_s = 10$. We take this as evidence that the dynamic dependence of the exchange-correlation kernel becomes more important with increasing coupling. Note that for small q , the DSF becomes narrow and the MEM estimate converges to the Bayesian prior. In particular, for $r_s = 100$ in Fig. 13, the DSF's peak is too narrow for our ω discretization.

A trimodal cross section is presented in Fig. 13 for $r_s = 100$ at $q = 1.4 k_F$. In context, we see from the error heatmaps in Fig. 11 that this q value is right on the border between where relative error is more than 50%; increasing q from 0, this curve is one of the first resolvable cross-sections. This raises suspicion about the trimodal peak. However, in Fig. 7, our investigation of a single exponential fit at small q and $r_s = 100$ showed that there is systematic deviation from the single exponential for $q = 1.4 k_F$, so we cannot say that the MEM procedure has produced clearly erroneous results. As such, we do not draw any conclusions from this trimodal cross section.

APPENDIX E: DSF SUM RULES FOR ALL r_s

For the interested reader, we plot in Fig. 14 the sum rules for all r_s not shown in the main text.

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