Stochastic Hamiltonians for correlated electron models

Frederick Green*
School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia

(Received 30 January 2019; published 25 June 2019)

Microscopically conserving reduced models of many-body systems have a long, highly successful history. Established perturbative theories of this type are the random-phase approximation for Coulomb fluids and the particle-particle ladder model for nuclear matter. There are also more physically comprehensive diagrammatic approximations, such as the induced-interaction and parquet models. Notwithstanding their explanatory power, some theories have lacked an explicit Hamiltonian from which all significant system properties, static and dynamic, emerge canonically. This absence can complicate evaluation of the conserving sum rules, essential consistency checks on the validity of any theory. In a series of papers Kraichnan introduced a stochastic embedding procedure to generate explicit Hamiltonians for common approximations for the full many-body problem. Existence of a Hamiltonian greatly eases the task of securing fundamental identities in such studies. I revisit Kraichnan's method to apply it to correlation theories for which such a canonical framework has been missing. I exhibit Hamiltonians for more elaborate correlated models incorporating both long-range screening and short-range scattering phenomena. These are relevant to the study of strongly interacting electrons and condensed quantum systems broadly.

DOI: 10.1103/PhysRevA.99.062118

I. INTRODUCTION

In the last century, within a remarkably brief span, the study of strongly correlated quantum systems witnessed a series of crucial innovations. The earliest example, for the electron fluid, is the random-phase approximation (RPA) of Pines and Bohm (see Refs. [1,2]), still a paradigm of many-body analysis today. Within the perturbative, or diagrammatic, philosophy the RPA was rapidly followed by formal developments from Martin and Schwinger [3], influencing the Green-function approach of Kadanoff and Baym (see Refs. [4,5]). Russian studies contributed in a major way [6], the Keldysh formalism [7,8] being the most familiar and in widespread use. Of the plentiful and thorough reference works surveying this vast area, we cite four standard texts by Pines and Nozières [2], Nozières [9], Rickayzen [10], and Mahan [11] and a more recent treatment by Coleman [12]. These provide a valuable cross section of different perspectives and analytic techniques.

The high-order perturbative models developed in this period, with their more specialized variants (as for superconductivity and superfluidity), offered tractable approximations beyond the long-ranged RPA to cover finer-scale, short-range correlations in condensed systems from the electron gas, to nuclear matter, to the helium fluids. The theories here in discussion are almost always cast in the language of Green functions and their dynamical equations.

Despite their technical ingenuity and effectiveness, many diagrammatic theories have had to be constructed bottom-up. A central conceptual tool has been missing by way of an explicit Hamiltonian underpinning. At times this has caused confusion around the interpretation of their dynamical sum rules (essential tests of the conservation laws), not to mention a level of *ad hoc* patchwork to try to fix these.

Amid these historical developments a canonical, top-down strategy for building model Hamiltonians was devised by Kraichnan [13,14], who turned his construction to the dominant correlation theories of the time. Kraichnan's stochastic approach to microscopic many-body dynamics revolutionized the different field of turbulence theory [15] although, while freely acknowledged to be of fundamental importance to correlated quantum systems [5], his innovation and its potential do not appear to have gained wide currency in the community. To this writer's mind it is an opportunity to be fully grasped; his sense is informed by an early and time-consuming effort to prove a higher frequency-moment sum rule for a correlated model of the electron gas [16]. It should really be enough to demonstrate the result once and for all and rely on the universality of the procedure. Knowing the Hamiltonian particular to an approximation would doubtlessly help.

Nondiagrammatic analyses have developed side by side with diagram-based ones and, as with the latter, they naturally start from a fundamental originating Hamiltonian. Two of the better-known nonperturbative approaches are density-functional theory [17,18] and the coupled-cluster formalism [19,20], but there, equally, a reduced Hamiltonian tailored to some model may not emerge on the path to a tractable approximation. Depending on which questions call for answers, as with diagrammatic theories, the lack of such a tool may have its disadvantages.

While the current paper is diagrammatically oriented, the model-Hamiltonian philosophy it adopts is wider than any specialized approach, with possible implications for nondiagrammatic approaches also. As an illustration one recalls the valuable insight of Jackson, Lande, and Smith [21] into the correspondence between a specific, nonperturbative variational model and a self-consistent diagrammatic one. In such

*frederickgreen@optusnet.com.au

a context the possibility of constructing a model Hamiltonian for one approximate description would immediately reflect upon the other.

In this paper I return to Kraichnan's methodology to show how it can be adapted readily to many-body formulations beyond the approximations analyzed by him, and for which an explicit Hamiltonian has not been available. The next section reviews the general method for building model Hamiltonians. It should be stressed that, while the focus will be on the uniform electron gas, Kraichnan designed the method to apply equally well to any system, finite or extended, with pair interactions. To establish familiarity with the approach, Sec. III revisits the classic approximations originally analyzed by him: the random-phase model, Hartree-Fock (HF), the ring approximation, and the particle-particle (Brueckner) ladder summation. Section IV introduces more complex operations for Hamiltonian models, both to single out RPA-related effects and long-range screening and then to unify them with strong ladder correlations dominant at short range. One such theory was applied by Green *et al.* [22], set up in part to understand angle-resolved inelastic x-ray scattering off metallic films [23]. Section V discusses two comprehensive theories of correlations: the maximally coupled parquet model [21,24–27] and a simplification of it, the induced-interaction approximation of Babu and Brown (see Refs. [28,29]) suited to such systems as nuclear matter and liquid helium, and extended later to low-density electron fluids [30]. The summary is given in Sec. VI.

Two Appendices follow the main body of the paper. Appendix A reviews the third frequency-moment sum rule in the electron gas as an example of how sum-rule validity, albeit generic to stochastic Hamiltonian models, also requires discretion when extracting the physical content of a reduced correlation theory. Appendix B looks briefly towards possible implications of the stochastic-Hamiltonian approach for nonperturbative analyses of correlated systems. As recalled above, these (in particular density-functional theory [17,18] and coupled-cluster analysis [19,20]) coexist with perturbative methods and likewise derive from an exact originating Hamiltonian. The potential for establishing explicit model structures for these alternative and powerful formulations of the quantum many-body problem could repay a thorough study.

II. STOCHASTIC HAMILTONIAN MODELS

A. Basic formulation

We begin with the standard Hamiltonian for a fermion system, comprising a single-particle part and an interaction part interacting via a pairwise potential:

$$H = \sum_k \epsilon_k a_k^* a_k + H_i,$$
$$H_i = \frac{1}{2}\sum_{k_1k_2k_3k_4}{}' \langle k_1k_2|V|k_3k_4\rangle a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4},$$
$$\langle k_1k_2|V|k_3k_4\rangle \equiv \delta_{s_1s_4}\delta_{s_2s_3} V(\mathbf{k}_1 - \mathbf{k}_4). \tag{1}$$

Notation is as follows. Index k denotes state wave vector $\mathbf{k}$ and spin s so a_k^* is the creation operator in state k and a_k is the annihilation operator; both satisfy the usual anticommutation relations. Here, the potential is spin independent. The summation $\sum'_{k_1k_2k_3k_4}$ comes with the momentum conservation restriction $k_1 + k_2 = k_3 + k_4$. In a uniform Coulomb system with neutralizing background, the terms in $V(\mathbf{0})$ are excluded.

The matrix element of the potential satisfies hermiticity and pairwise exchange symmetry:

$$\langle k_4k_3|V|k_2k_1\rangle = \langle k_1k_2|V|k_3k_4\rangle^*,$$
$$\langle k_2k_1|V|k_4k_3\rangle = \langle k_1k_2|V|k_3k_4\rangle. \tag{2}$$

The Hamiltonian presented is assumed exact for the system of interest. The first step in the Kraichnan construction is to posit a large number N of Hamiltonians identical to that of Eq. (1) but the fermion states of which are distinguishable. In other words, an additional N-fold spinlike label is assigned to each system. We form the total Hamiltonian for the assembly:

$$\mathcal{H}_N = \sum_{n=1}^{N}\sum_k \epsilon_k a_k^{*(n)} a_k^{(n)} + \frac{1}{2}\sum_{n=1}^{N}\sum_{k_1k_2k_3k_4}{}' \langle k_1k_2|V|k_3k_4\rangle\, a_{k_1}^{*(n)} a_{k_2}^{*(n)} a_{k_3}^{(n)} a_{k_4}^{(n)}; \tag{3}$$

the additional superscript n distinguishes the populations.

Next we map the assembly in Eq. (3) to a "collective" description. This is done by canonically transforming the operators into a complementary set over the large, but still finite, space N. For integer $\nu \leqslant N$ introduce

$$a_k^{*[\nu]} \equiv N^{-1/2}\sum_{n=1}^{N} e^{2\pi i\nu n/N} a_k^{*(n)} \quad \text{and}$$
$$a_k^{[\nu]} \equiv N^{-1/2}\sum_{n=1}^{N} e^{-2\pi i\nu n/N} a_k^{(n)} \tag{4}$$

with the usual Fourier-series convention that sums of collective indices ν are defined modulo N. The collective operators of Eq. (4) satisfy the same anticommutation relations as the original operators. The total Hamiltonian becomes

$$\mathcal{H}_N = \sum_{\nu=1}^{N}\sum_k \epsilon_k a_k^{*[\nu]} a_k^{[\nu]} + \frac{1}{2N}\sum_{k_1k_2k_3k_4}{}' \sum_{\nu_1\nu_2\nu_3\nu_4}^{N} \delta_{\nu_1+\nu_2,\nu_3+\nu_4} \times \langle k_1k_2|V|k_3k_4\rangle\, a_{k_1}^{*[\nu_1]} a_{k_2}^{*[\nu_2]} a_{k_3}^{[\nu_3]} a_{k_4}^{[\nu_4]}. \tag{5}$$

B. Stochastic ansatz

The ground is ready for Kraichnan's procedure. The object described by Eq. (5) remains in every respect the exact Hamiltonian, merely replicated N times in distinguishable but otherwise identical Hilbert spaces. Within its new collective representation, however, it is possible to modify the interaction by introducing couplings specifically tailored to enhance certain classes of correlated expectation values, suppressing the remainder. In the process the modified collective Hamiltonian retains its functional properties.

All of the Hilbert-space machinery and the consequences from the fundamental equation of motion continues to apply to the collective Hamiltonian. After ensemble averaging, those identities particularly determined by analyticity of the expectation values will survive averaging, since their causal structure is preserved. More care is needed with any identities that depend explicitly on completeness in Hilbert space, which may not survive averaging. This is discussed in Appendix A.

Following Kraichnan we define restriction variables $\varphi_{\nu_1\nu_2|\nu_3\nu_4}$ to adjoin to the interaction potential. The ensemble interaction Hamiltonian becomes

$$\mathcal{H}_{i;N} = \frac{1}{2N}\sum_{k_1k_2k_3k_4}{}' \sum_{\nu_1\nu_2\nu_3\nu_4}^{N} \delta_{\nu_1+\nu_2,\nu_3+\nu_4}\varphi_{\nu_1\nu_2|\nu_3\nu_4} \times \langle k_1k_2|V|k_3k_4\rangle a^{*[\nu_1]}_{k_1}a^{*[\nu_2]}_{k_2}a^{[\nu_3]}_{k_3}a^{[\nu_4]}_{k_4}. \quad (6)$$

To maintain the hermiticity and label symmetry of V itself, the parameter $\varphi_{\nu_1\nu_2|\nu_3\nu_4}$ must satisfy its corresponding form of Eq. (2), noting that the collective creation and annihilation operators in Eq. (6) bind together the collective labels ν_j and system basis-state labels k_j for $j = 1, 2, 3, 4$.

The properties of V shared by φ are crucial to the entire exposition. They establish the microscopic equivalence of the Kraichnan procedure to the Baym-Kadanoff rules [4,5] for constructing conserving, or "Φ-derivable," models of the interacting free-energy functional. Given these constraints, the introduced variable will couple the formerly independent Hamiltonian components in any way one wishes without upsetting the analytic structure of the N-fold system. In particular, they can be assigned randomly determined values.

When the choice of φ is not random, the consequences are immediately reflected in the N-fold Hamiltonian. When the choice is random the Hamiltonian, altered in this way, is to be embedded within a still larger ensemble. Each member of this supercollection has an identical form in terms of the restriction parameters but each is characterized by its own specific set of stochastic values. Depending on the restrictions' internal structure, certain products of them will cancel within the diagrammatic expansion of the ground-state energy. These terms are the subset of correlations designed to survive the final ensemble averaging over the assigned value of φ. All other terms will tend to interfere destructively, to be quenched in the ensemble average.

Thus Kraichnan's calculational philosophy is exactly that of Bohm and Pines's RPA, albeit far more flexible. In principle, such a construct is able to generate models with a vast range of selected perturbation terms—to all orders when required—naturally dictated by the physical context to be captured. The selection is expressed through the particular restrictions imposed via φ.

Every such implementation is a truncation to the complete many-body problem, although the truncation can be very sophisticated. Throughout the reduction, each model still possesses a well-defined Hamiltonian ensemble respecting—in its own reduced fashion—all of the relevant analytic identities, and their inter-relationships, inherent in the exact description. Quantitatively, of course, the changes might be drastic while, qualitatively, the generic behavior and development of the system under its Hamiltonian will always apply. The power of the approach consists precisely in this.

Before reviewing classic examples of reduced Hamiltonians (including from the original Kraichnan study) and going on to different and more comprehensive correlation models, we recapitulate the procedural logic.

(1) Conceptualize a sufficiently large number N of dynamically identical, but distinguishable, copies of an exact Hamiltonian. Each retains the same interaction potential but all copies are mutually uncoupled. This enlarged Hamiltonian exhibits physics completely identical to any one of the embedded copies of the exact system.

(2) Fourier transform the state operators of each copy to a new set of operators for a coherent pseudocollective superposition of the N systems. The transformation generates a new set of indices, formally analogous to the wave-vector states in reciprocal space.

(3) For the pseudocollective description, introduce a set of restriction factors labeled by the new collective indices. Adjoin each factor to the basic (unaffected) interaction potential.

(4) The functional form of the factor must satisfy the same label symmetries as does the potential with respect to its state labels. This is equivalent to the Baym-Kadanoff rules [4,5] and preserves the modified Hamiltonian as a Hermitian operator, with all the canonical identities also preserved.

(5) The N copies are now interlinked via the introduced factors, and these couplings can be assigned values within any desired protocol; in particular, they may be defined stochastically.

(6) Finally, ensemble average the system over the distribution governing the coupling factors. Since each parametrized N-fold Hamiltonian retains its fundamental properties, analytic relations among expectation values will be preserved functionally—but not usually numerically—after averaging.

The central element is to have made sure that all such model Hamiltonians retain the analytic characteristics of the original physical Hamiltonian. To establish quantitative results from the model, one simply follows the same theoretical steps applicable to the exact system. This is of enormous help in confirming microscopic conservation for any model, notably through the dynamical sum rules that condition its response and fluctuation structure [2].

Whether or not the resulting numbers are adequate to the physical situation one wants to analyze depends strictly on how the ensemble parameters φ are chosen, just as in the more directly intuitive and synthetic Φ-derivable approach [4,5]. Nevertheless, certain basic inner relationships such as sum rules among derived quantities remain valid throughout.

III. INSTANCES OF MODEL HAMILTONIANS

We preface the later extension of Kraichnan's construction to other many-particle model systems by reviewing the classic examples. We first introduce the RPA model before revisiting the classic formulations first analyzed by Kraichnan.

A. Random-phase approximation

The Bohm-Pines RPA can be obtained by defining its variable as

$$\varphi^{\rm RPA}_{\nu_1\nu_2|\nu_3\nu_4} = \delta_{\nu_1\nu_4}\delta_{\nu_2\nu_3}. \quad (7)$$

This nonrandom assignment fulfils the symmetries of Eq. (2). Its effect is illustrated in Fig. 1 via its contributions to the ground-state correlation-energy functional. In a many-body system, only "linked" diagrams, namely, those consisting of

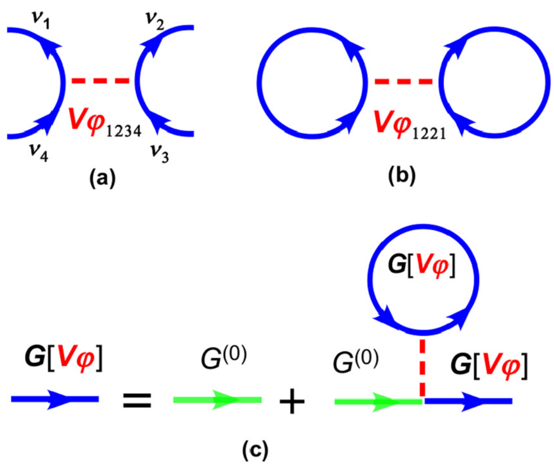

FIG. 1. Structure of the random-phase approximation, or RPA. Continuous lines, incoming or outgoing particle; broken lines, interaction. The restriction parameter $\varphi^{\rm RPA}$ of Eq. (7) generates the coupling shown in (a). Successive interaction terms in the Hamiltonian cannot interlink through this parameter. Only the single linked diagram shown in (b) survives to define the ground-state correlation energy. Given the Hamiltonian, the Dyson equation, symbolized in (c), can be set up directly for the RPA single-particle Green function $G[V\varphi]$ starting from the noninteracting Green function $G^{(0)}$. Although the RPA correlation energy has the simplest possible structure of any model, the high level of self-consistency is evident through the structure of the Dyson equation (c).

a single diagrammatic unit, represent valid contributions to the correlation energy [5]. The object that results from the prescription in Eq. (7) is just the direct Hartree (or mean-field) correlation energy, Fig. 1(b). All other would-be contributions to higher order in $V\varphi$ that do not vanish identically turn out to be unlinked in the summation over indices, and therefore do not enter into the canonical correlation-energy functional.

When the Hamiltonian is augmented with an external perturbation, the associated Heisenberg equation of motion [11] leads systematically to both one-body and two-body dynamical Green functions, or propagators. These contain the necessary information for computing those response functions that can be compared with experimental measurements. Figure 1(c) shows the prototypical Dyson integral equation [11] for the one-body propagator within the RPA entering into the energy functional of Fig. 1(b). Notwithstanding the structural simplicity of the random-phase approximation, this reveals the high degree of internal nesting that lies implicitly concealed within it, as with any nontrivial theory of many-body correlations.

B. Hartree-Fock

The next simplest model is HF, which introduces the primary exchange corrections to the RPA. In place of Kraichnan's own choice for selecting the Hartree-Fock Hamiltonian, we adapt the same ansatz as for RPA after antisymmetrizing the original pair interaction following Nozières [9]. This is done by exchanging one pair of incoming or outgoing indices, say $3 \leftrightarrow 4$ for definiteness, and using anticommutation to

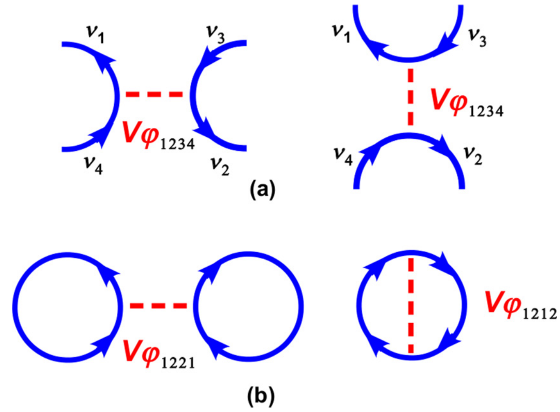

FIG. 2. Correlation diagrams associated with the model Hamiltonian carrying the Kraichnan RPA factor $\varphi^{\rm RPA}_{\nu_1\nu_2|\nu_1\nu_2}$ [see Eq. (7)] now with exchange explicitly incorporated in the interaction potential. The allowed topological possibilities for the two-body vertex are shown in (a). The only linked diagrams to survive the trace over $\varphi^{\rm RPA}$ are those of (b), exhibiting the standard Hartree and Fock exchange-correlation energy terms. With the potential antisymmetrized, each of the vertices of (a) will contribute half of the total direct and exchange terms of (b). (Combinatorial weightings for the correlation diagrams will not be shown; they are identical to the standard derivation of the ground-state functional [4].)

replace $\langle k_1k_2|V|k_3k_4\rangle$ with

$$\langle k_1k_2|\overline{V}|k_3k_4\rangle \equiv \tfrac{1}{2}(\langle k_1k_2|V|k_3k_4\rangle - \langle k_1k_2|V|k_4k_3\rangle) \quad (8)$$

in the full Hamiltonian. It makes no change to the physics, but means that the RPA ansatz Eq. (7) also covers the exchange vertex as in Fig. 2(a). The outcome is the Hartree correlation energy of Fig. 1(b) once again, now accompanied by its Fock exchange counterpart. In a Coulomb system, the long-ranged effects remain subsumed under the Hartree structure. At shorter range, comparable to the system's Fermi wavelength, the Fock term corrects for Pauli repulsion, which is absent from RPA causing it to overestimate the Coulomb energy.

C. Shielded interaction

The first truly stochastic ansatz introduced by Kraichnan regenerates the shielded-interaction, or "ring," approximation [4] closely related to but richer than the pure RPA and HF. In a system with long-ranged potential, it provides the leading short-range correlation corrections to the screening properties of the system. For the ring model, the restricting factors are defined in terms of a uniform random distribution of phase angles so that

$$\varphi^{(r)}_{\nu_1\nu_2\nu_3\nu_4} \equiv \exp\left[\pi i\big(\zeta_{\nu_1\nu_4} + \zeta_{\nu_2\nu_3}\big)\right], \quad \zeta_{\nu\nu'} \in [-1, 1];$$
$$\zeta_{\nu'\nu} = -\zeta_{\nu\nu'}. \quad (9)$$

The phase reverses when the roles of an outgoing and incoming pair of lines reverse (particle $\leftrightarrow$ hole). Kraichnan's choice of a phase ansatz always follows a possible action of the local particle operators (creation and annihilation) inside the diagrammatic structures one wants to highlight. Here, $\zeta_{\nu\nu} \equiv 0$ for a self-closing line.

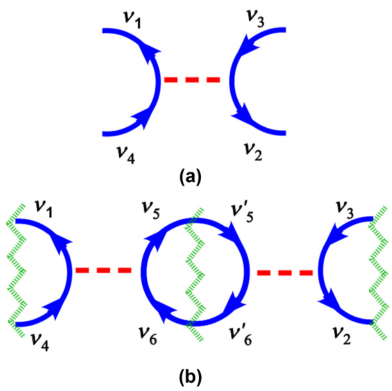

FIG. 3. Allowed vertex contributions for the RPA stochastic Hamiltonian model [see Eq. (9)]. (a). Lowest-order (Hartree) term. (b). All other surviving terms can only adopt a repeated chain-link topology. The outer open lines of all terms may link in two different ways, leading either to open chains or simple rings.

Consider Fig. 3(b) to second order in the interaction. Closing the intermediate lines enforces equality of the intermediate pairs ν_5, ν_5' and ν_6', ν_6 to form an elementary particle-hole polarization "bubble." The concatenation $\varphi_{\nu_1\nu_5|\nu_6\nu_4}\varphi_{\nu_6\nu_2|\nu_3\nu_5}$ then leads to the net phase

$$(\zeta_{14}+\zeta_{56})+(\zeta_{65}+\zeta_{23})=\zeta_{14}+\zeta_{23}. \tag{10}$$

It is clear that the cancellation observed in Eq. (10) persists to all orders in the ground-state diagram expansion. This secures the survival of the chainlike terms. For any other topology the phases will not cancel and will thus be suppressed in the trace over the stochastic ensemble.

An illustrative example of correlated terms surviving the ensemble average for the ring model appears in Fig. 4 where we display its associated density-density response, or polarization, function [2]. In the momentum-frequency domain the characteristically screened interaction, as defined in Fig. 4(c), pairs the lowest-order polarization $\chi(q,\omega)$ with the bare potential $V(q)$. The summation runs to all orders, but *only* for those components allowed by the parameter Eqs. (9) and (10).

D. Particle-particle ladder

The ring model builds upon the RPA/HF by incorporating the next level of screening corrections at finite range, but does not do well for shorter-ranged interactions with a hard core, such as nucleons or neutral atomic fluids where the extreme degree of local repulsion between particles invalidates the finite-order Born approximation [28]. Accounting for hard-core effects requires the ladder approximation of Brueckner and Gammel [32], designed to accommodate the extreme distortion in the pair-correlation function from the interaction at close range. The aim is to incorporate the full Born series for two-particle scattering in the interacting medium, using the Bethe-Salpeter equation [9].

Following Kraichnan, the ladder-model Hamiltonian is defined by the restriction parameter

$$\varphi^{(pp)}_{\nu_1\nu_2|\nu_3\nu_4}\equiv\exp\left[\pi i\left(\xi_{\nu_1\nu_2}-\xi_{\nu_3\nu_4}\right)\right],\quad \xi_{\nu\nu'}\in[-1,1];$$
$$\xi_{\nu'\nu}=\xi_{\nu\nu'}. \tag{11}$$

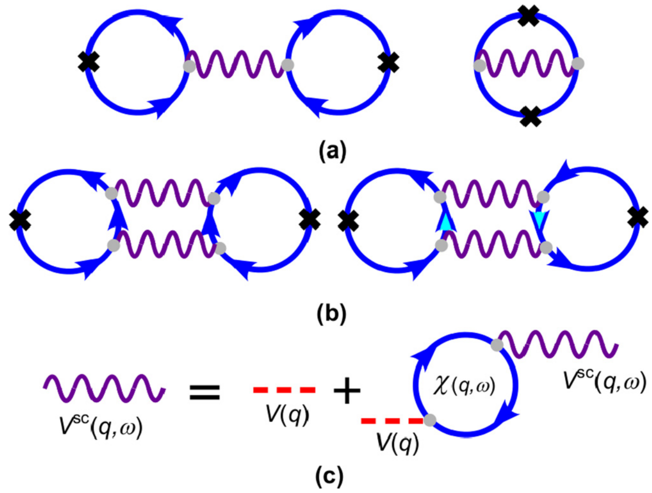

FIG. 4. Topology of the correlation corrections to the density-density response function in the stochastic ring model. Crosses denote coupling to an external perturbation of the density. Screened Hartree-Fock contributions appear in (a) while (b) shows a new pair of correlated contributions necessarily appearing in the response to satisfy microscopic conservation at the two-body level [4,31]; note that they are functionally distinguished by the mutual orientation of their attached loops: in the left-hand term the screened potentials are connected by two particle lines while in the right-hand term they are connected by a particle and a hole. The intermediate propagators for these processes act differently. In (c) the equation for the self-consistent screened interaction of (a) and (b) is defined. The object $\chi(q,\omega)$ is the leading term in the total polarization response.

While $\varphi^{(r)}$ for the ring model favors particle-hole pair propagation via polarization bubbles, $\varphi^{(pp)}$ for the ladder approximation privileges two-particle propagation mediated not by the bare interaction but by its complete pairwise scattering matrix. This is shown in Fig. 5. When the restriction factors are concatenated as with Eq. (10) of the ring model, this time the pattern for the sum of phases is

$$\left(\xi_{\nu_1\nu_2}-\xi_{\nu_3'\nu_4'}\right)+\left(\xi_{\nu_1'\nu_2'}-\xi_{\nu_3\nu_4}\right)=\xi_{\nu_1\nu_2}-\xi_{\nu_3\nu_4} \tag{12}$$

since the algebra of creation-annihilation pairing now forces $\nu_1'=\nu_4'$ and $\nu_2'=\nu_3'$. From Eq. (12) the same cancellation obtains under exchange $\nu_1'=\nu_3'$ and $\nu_2'=\nu_4'$, leading to a contribution analogous to the Fock term in the ground-state correlation energy. Figure 6 illustrates the polarization corrections expected within the ladder approximation.

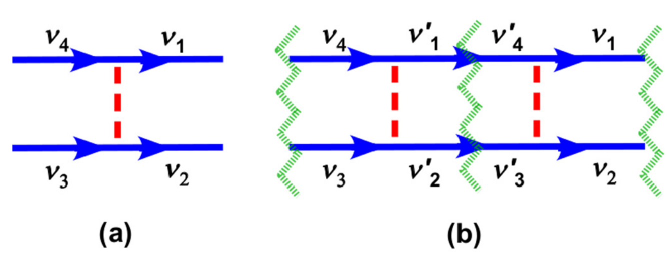

FIG. 5. Repeated sequences, or ladders, of particle-particle dynamical correlations with the stochastic restriction parameter of Eq. (11). The elementary scattering term is in (a) while in (b) all stochastic phases of inner propagator pairs cancel in all higher orders.

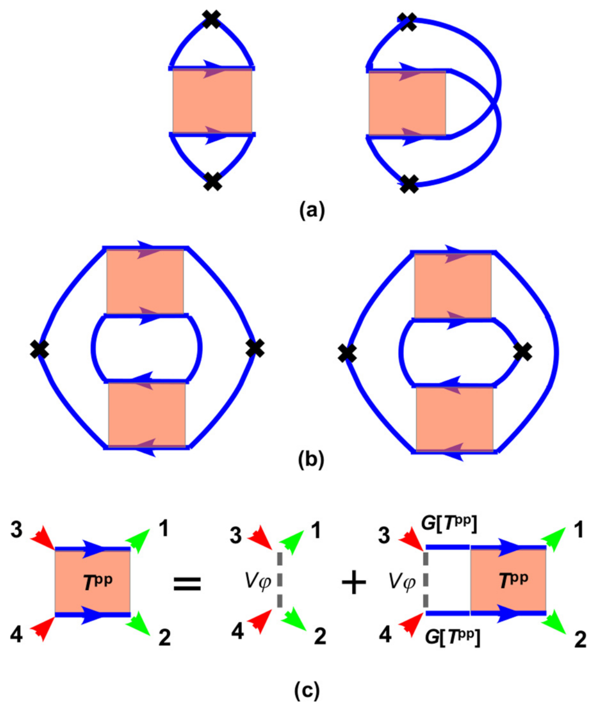

FIG. 6. Irreducible corrections to the polarization response in the particle-particle ladder approximation. These are obtained, as for the ring model, by a standard variational procedure starting from the many-body ground-state functional. Diagrams in (a) carry a single particle-particle ladder-scattering vertex. Note that the exchange term on the right of (a) is already accounted for within the term on the left and is presented merely to bring out the internal topology of this contribution. Diagrams in (b) display the two possibilities (a consequence of conservation [4]) by which the particle-particle amplitude also mediates intermediate particle-hole processes. The Bethe-Salpeter equation for the scattering vertex, or particle-particle T matrix T^{pp}, is schematized in (c). The single-particle propagator is similarly self-consistently defined by T^{pp} through the Dyson equation for the model.

E. Particle-hole ladder

The particle-hole ladder model extends the exchange structure of Hartree-Fock in the way that the ring model does for the direct random-phase approximation. This particular scattering channel will be needed in Sec. V. With a slight change to the particle-particle mechanism, we generate its particle-hole analog. Consider

$$\varphi^{(ph)}_{\nu_1\nu_2|\nu_3\nu_4} \equiv \exp\left[\pi i\left(\vartheta_{\nu_1\nu_3} + \vartheta_{\nu_2\nu_4}\right)\right], \quad \vartheta_{\nu\nu'} \in [-1, 1]; \quad \vartheta_{\nu'\nu} = -\vartheta_{\nu\nu'}. \tag{13}$$

Particle-hole pairings in the elementary interaction vertex are coupled as if the hole were a particle; reversing the roles in the pair reverses their phase, as one would expect. The leading corrections to the polarization for the particle-hole ladder model, analogous to those of Fig. 6 for the particle-particle ladder, are in Fig. 7 including the terms of Fig. 7(b) of second order in the total scattering amplitude and required by conservation.

This ends the review of the Hamiltonian formulations first presented by Kraichnan for standard correlation models. We have added the random-phase approximation in its own right (otherwise subsumed by Kraichnan under his Hartree-Fock prescription) as well as the particle-hole ladder. In the following section we explore more comprehensive Hamiltonian models.

IV. EXTENSIONS OF KRAICHNAN'S METHOD

A. Systematic removal of correlations: Screened Hamiltonian

We start by posing the problem of how an interacting Hamiltonian may change when certain components are removed selectively, as one would do for closer analysis of the remnant correlations. As an example we isolate the RPA Hamiltonian from the exact description. There is no loss of physical content in recasting Eq. (5) as

$$\mathcal{H} = \mathcal{H}^{\rm RPA} + \frac{1}{2N}\sum_{\ell_1\ell_2\ell_3\ell_4} \delta_{\ell_1+\ell_2,\ell_3+\ell_4}\left(1 - \varphi^{\rm RPA}_{\nu_1\nu_2|\nu_3\nu_4}\right) \langle k_1k_2|V|k_3k_4\rangle a^*_{\ell_1}a^*_{\ell_2}a_{\ell_3}a_{\ell_4} \ \text{ where}$$

$$\mathcal{H}^{\rm RPA} = \sum_{\ell} \epsilon_k a^*_\ell a_\ell + \frac{1}{2N}\sum_{\ell_1\ell_2\ell_3\ell_4}{}' \varphi^{\rm RPA}_{\nu_1\nu_2|\nu_3\nu_4} \langle k_1k_2|V|k_3k_4\rangle a^*_{\ell_1}a^*_{\ell_2}a_{\ell_3}a_{\ell_4}. \tag{14}$$

To streamline the notation from now on, in the second expression of Eq. (14) we have grouped the joint variables $\{k, \nu\}$ in $a^{[\nu]}_k$ into one symbol ℓ so $a^{[\nu]}_k \equiv a_\ell$. Summations over ℓ encompass summations over both k and ν; Kronecker deltas are now products of those in ks and νs and, again, $\sum'_{\ell_1\ell_2\ell_3\ell_4}$ is under the constraint $\ell_1 + \ell_2 = \ell_3 + \ell_4$ standing in for $k_1 + k_2 = k_3 + k_4$ and $\nu_1 + \nu_2 = \nu_3 + \nu_4$.

So far nothing has changed; nor is there loss of any formal attribute on introducing the reduced RPA-free version

$$\mathcal{H}^{\rm sc}[\psi] \equiv \sum_\ell \epsilon_k a^*_\ell a_\ell + \frac{1}{2N}\sum_{\ell_1\ell_2\ell_3\ell_4}{}' \left(1 - \varphi^{\rm RPA}_{\nu_1\nu_2|\nu_3\nu_4}\right) \psi_{\nu_1\nu_2|\nu_3\nu_4} \langle k_1k_2|V|k_3k_4\rangle a^*_{\ell_1}a^*_{\ell_2}a_{\ell_3}a_{\ell_4} \tag{15}$$

as long as the restriction parameter ψ has the symmetries required by Eq. (2).

The object in Eq. (15) represents all the correlations of physical interest *except* for the collective plasmon mode [2]. In the language of Bohm and Pines this is the Hamiltonian for the screened assembly: the part responsible for the near-field dynamics experienced by a test particle immersed in the system.

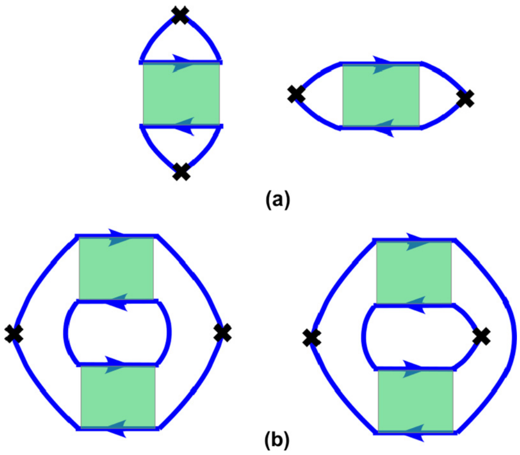

FIG. 7. Irreducible polarization corrections for the particle-hole ladder interaction associated with Eq. (13). Diagrams in (a) carry a single ladder-scattering vertex. Diagrams in (b) display the two additional topological possibilities in which the vertex also mediates intermediate particle-hole propagation within the polarization function. The Bethe-Salpeter equation for the particle-hole ladder is essentially that for particle-particle scattering except that one set of particle lines is reversed and exchange is excluded.

First and foremost the screened Hamiltonian $\mathcal{H}^{sc}$ has experimental relevance to metallic electron systems in the normal state, since an external magnetic field will couple to the spin density but not to the total charge density. In this situation RPA screening does not contribute.

Besides this essential practical application, the theoretical relevance of separating out the random-phase part is for the sum rules. We illustrate the case of the f-sum rule, a familiar identity expressing particle and energy conservation. Its proof (see, for example, Nozières [9]) relies on the fact that the time-dependent operator in the Heisenberg picture [11],

$$\rho_{\ell\ell'}(t,t') \equiv a^*(t)_\ell a_{\ell'}(t'),$$

commutes with any pairwise interaction Hamiltonian—exact or reduced—as long as the same label symmetries of the interaction are satisfied both in physical and in Kraichnan's pseudocollective spaces.

The f-sum rule connects the net energy absorbed from an external perturbation to the energy distribution among the available excitations of the system. In the classic case of the uniform electron gas at zero temperature, it states (adopting units in which $\hbar$ and the free-electron mass are set to 1)

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\omega S(q,\omega) = \frac{q^2}{2}n, \tag{16}$$

in which q is the momentum transferred by the perturbation and n is the electron density. The dynamic structure factor $S(q,\omega)$ is the density of states for all the system's excited modes at momentum energy (q,ω); it is the negative imaginary part of the total dynamic polarization $\chi(q,\omega)$, including the contribution from the collective plasmon mode.

Proof of the f-sum rule follows from the dynamical equations for $\rho_{\ell\ell'}$ governed by the Hamiltonian. The rule asserts that, no matter how the absorbed energy is redistributed throughout the perturbed system (in more or less intricate ways), in sum it is conserved and must account for the energy gained per particle. The question is: does the electron gas have an analogous rule when the dominant plasma mode is "removed" in a sense to be made precise?

The answer to the above is yes. This is almost obvious, since the right-hand side of Eq. (16) has no dependence on the interaction (and consequently is insensitive to all internal correlations and all modifications to the potential that do not alter its symmetries). In this form the rule is known commonly as the conductivity sum rule.

One knows already that any canonical derivation for the full Hamiltonian, for instance, the f-sum rule, will be valid for a reduced Hamiltonian. The logical form of such a proof, once given for the exact case, does not care about the nature of any appropriate reduction. Accordingly, let $S^{sc}(q,\omega)$ be the dynamic structure factor appropriate to $\mathcal{H}^{sc}[\psi]$ of Eq. (15). If we now perturb this system, conservation nevertheless applies and we obtain

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\omega S^{sc}(q,\omega) = \frac{q^2}{2}n, \tag{17}$$

or the conductivity sum rule, with essentially zero effort.

The Hamiltonian system $\mathcal{H}^{sc}[\psi = 1]$ preserves all non-RPA contributions to the true ground state. This is because its one-body propagators are unchanged by screening as the Hartree mean-field term in the self-energy [11] is always canceled by local charge neutrality. For nonuniform Coulomb systems this is not true in general, but in the uniform situation the polarization $\chi^{sc}(q,\omega)$, the imaginary part of which is $-S^{sc}(q,\omega)$, contains only the "proper" correlations for the original system, that is, all those that are not RPA. In that sense the system becomes formally shielded from its long-range physics. The consequent ability to validate sum-rule consistency for any screened reduced model is of central importance; while Eq. (17) then conveys no additional physical information, it does provide an essential numerical test in implementing models of the uniform electron fluid.

B. Systematic addition of correlations: Ring-plus-ladder model

In the previous section we discussed two paradigms: the ring model, which improves upon Hartree-Fock by including some shorter-ranged correlations from the screened interaction (RPA, essentially), and the particle-particle ladder model to treat strong short-ranged effects beyond exchange. A combination of both was implemented by Green, Neilson, and Szymański [22] for the electron gas to interpolate between dominant long-range Coulomb screening and the short-range Coulomb correlations expected to prevail at wavelengths accessible in high-energy x-ray scattering [23].

The long-range-with-short-range interpolation was built bottom-up, as it were, by isolating its physically dominant diagrams, the rings and ladders of Figs. 4 and 6, out of the expansion of the exact ground-state correlation energy. These terms were duly symmetrized to make sure that they obeyed the Baym-Kadanoff criteria for conserving, or Φ-derivable, approximations [4,5].

Typical of Φ-derivable theories, the ring-plus-ladder model was set up without a Hamiltonian, rendering subsidiary derivations more burdensome than they might have been. Here we present a stochastic Hamiltonian for the Green *et al.* [22]

prescription:

$$\mathcal{H}^{\rm GNS} \equiv \sum_{\ell} \epsilon_k a^*_\ell a_\ell + \frac{1}{2N} \sum_{\ell_1\ell_2\ell_3\ell_4} \varphi^{\rm GNS}_{\nu_1\nu_2|\nu_3\nu_4} \langle k_1k_2|V|k_3k_4\rangle a^*_{\ell_1} a^*_{\ell_2} a_{\ell_3} a_{\ell_4},$$

$$\varphi^{\rm GNS}_{\nu_1\nu_2|\nu_3\nu_4} \equiv 1 - \big(1-\varphi^{(r)}_{\nu_1\nu_2|\nu_3\nu_4}\big)\big(1-\varphi^{(pp)}_{\nu_1\nu_2|\nu_3\nu_4}\big) = \varphi^{(r)}_{\nu_1\nu_2|\nu_3\nu_4} + \varphi^{(pp)}_{\nu_1\nu_2|\nu_3\nu_4} - \varphi^{(r)}_{\nu_1\nu_2|\nu_3\nu_4}\varphi^{(pp)}_{\nu_1\nu_2|\nu_3\nu_4}, \tag{18}$$

where the restriction parameters $\varphi^{(r)}$ and $\varphi^{(pp)}$ are those defined stochastically for rings, Eq. (9), and for particle-particle ladders, Eq. (11). Hence the reduced interaction for this hybrid meets Kraichnan's conditions on label symmetry.

The effect of combining distinct classes of interaction in this way is readily seen. When either class of phase factor survives, its counterpart will not. If both combinations do survive (as in the polarization to first and second order in the interaction) there is no duplication. Their physics acts cooperatively in the total correlation behavior, though never concurrently.

Diagrammatically, whether for the exact or any approximate Hamiltonian, the functional $\Phi[\varphi V]$ for the correlation energy is read off directly as the expectation of the interaction part of the Hamiltonian. This involves the self-energy $\Sigma[\varphi V; G]$, where $G[\varphi V]$ is the self-consistent one-body propagator, or Green function. Φ and Σ are related in two ways. The first is via the Hellmann-Feynman integral identity [2]: the underlying pair interaction V is multiplied by a coupling constant taken from zero to unity so

$$\Phi[\varphi V] \equiv \frac{1}{2}\int_0^1 \frac{dz}{z} \sum_\ell \langle G_{-\ell}[z\varphi V]\Sigma_\ell[z\varphi V; G]\rangle \tag{19}$$

in which the self-energy and propagator within the right-hand integrand are evaluated at the coupling constant z. The second relation complementary to Eq. (19) is the variational derivative [5]

$$\Sigma_\ell[\varphi V; G] = \frac{\delta\Phi[\varphi V]}{\delta G_{-\ell}}. \tag{20}$$

The generic structure of $\Phi[\varphi V]$, whether exact or associated with a Kraichnan Hamiltonian or to its functional equivalent, Φ derivability [4,5], has a very specific property. Within the expansion of the exact Φ in powers of the underlying potential partnered by the fully renormalized propagators G within the description, each G "sees," that is, is embedded in, a correlation environment identical to any other propagator in the given term [5]. It must not matter which G is removed to generate the self-energy diagrams for the relation Eq. (20). The same Σ must emerge. Were the above not the case, Σ would lack the symmetry needed for conservation. Since its symmetry ultimately comes from the Hermitian nature of the Hamiltonian, it follows *a priori* and with no extra work that every stochastic Hamiltonian model must possess a family of terms making up Φ with the same symmetries as those that secure microscopic conservation in the exact case. This brings home the analytic power of Kraichnan's procedure.

Figure 8 illustrates the consequences of the Hamiltonian Eq. (18) for the self-energy given by Eq. (20). Self-consistency of the one-body Green function through the self-energy leads to the implicit nesting of rings and ladders to all orders in the interaction. Nevertheless there can be no ladders with chainlike rungs; they are stochastically suppressed.

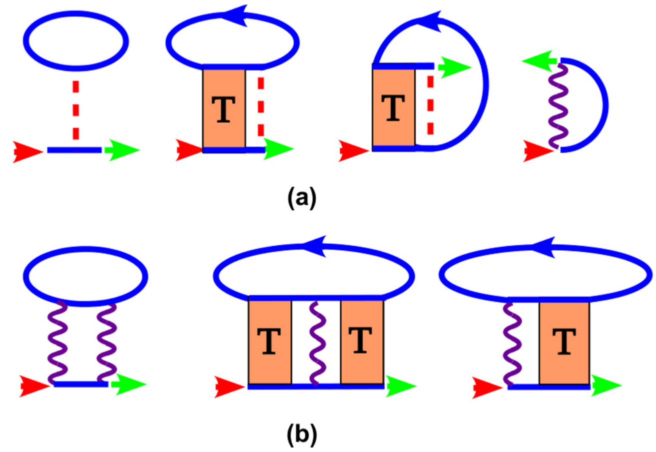

FIG. 8. Structure of model self-energy for the interpolating rings-plus-ladders model. Allowed contributions appear in (a). Other combinations, of which those in (b) are instances, are inhibited in the stochastic average.

The diagrams that survive stochastic filtering are just those of the Green *et al.* prescription [22]. Its polarization corrections to leading order in the particle-particle T matrix comprise the sum of the terms in Figs. 4 and 6, compensated for overcounting. Overcounting is automatically excluded in Eq. (18) while in any constructive Φ-derivable model—that of Ref. [22] is just one instance—overcounting must be corrected by hand because the choice of a correlation subset, while obviously physically guided, is still a matter of piece-by-piece selection out of the full ground-state expansion.

Equation (18) furnishes the prototype for the similarly motivated but more intricate approximations in the next section. With a proper Hamiltonian, treatment of various sum rules in this model becomes much more efficient. The point is made in Appendix A, in which the third frequency-moment sum rule is recalled and interpreted in terms applicable to all models.

Having introduced the notion of selective combination of disparate physical correlations within a unified Hamiltonian, we are ready for the more comprehensive parquet and induced-interaction series. Particularly in nuclear-matter and liquid-helium studies, these distinguish topologically among particle-particle ladder processes, sequential RPA-like polarization processes, and the latter's exchange counterparts the particle-hole ladders. All three stochastic components are available.

V. PARQUET AND THE INDUCED INTERACTION

We end this paper with the discussion of Hamiltonians for approximate theories based on a maximal inclusion of strictly pairwise correlations, starting with the parquet theory. It has long been appreciated that not all correlations in the many-body ground state are representable as structures made up purely from sequential two-body scatterings. Irreducible processes contribute that do not fit, topologically, the templates covered above [21]. Absent a general procedure to include these, practical modeling efforts emphasized incorporating all possible contributions reducible to the standard pair processes.

A. Parquet Hamiltonian

The most elaborate attempt at constructing a comprehensive theory purely out of two-body processes is parquet. A further significant feature of parquet is its intimate connection with variational methods offering nonperturbative calculational approaches to strong-correlation problems [21,25]. The conceptual advantages of knowing its Hamiltonian would go beyond the immediate precincts of diagrammatic theory.

The parquet diagrams include all those that, to all orders, would tile the entire plane in systematic patterns, hence their name. The ingredients for its Hamiltonian are at our disposal via the only possibilities for two-body scattering: rings and the two species of ladder, particle-particle and particle-antiparticle. The parquet Hamiltonian is proposed to be

$$\mathcal{H}^{\rm pqt} = \sum_{\ell} \epsilon_k a_\ell^* a_\ell + \frac{1}{2N}\sum_{\ell_1\ell_2\ell_3\ell_4} \varphi^{\rm pqt}_{\nu_1\nu_2|\nu_3\nu_4} \langle k_1k_2|V|k_3k_4\rangle a^*_{\ell_1} a^*_{\ell_2} a_{\ell_3} a_{\ell_4},$$

$$\varphi^{\rm pqt}_{\nu_1\nu_2|\nu_3\nu_4} \equiv 1 - \left(1-\varphi^{(r)}_{\nu_1\nu_2|\nu_3\nu_4}\right)\left(1-\varphi^{(ph)}_{\nu_1\nu_2|\nu_3\nu_4}\right)\left(1-\varphi^{(pp)}_{\nu_1\nu_2|\nu_3\nu_4}\right). \tag{21}$$

It is a generalization of the cooperative, yet strictly sequential, structure of restriction factors in the rings-plus-ladders Hamiltonian of the previous section, Eq. (18). It manifestly allows for all possible planar topologies produced by pairwise scatterings in maximally complex combinations but not getting in one another's way, thereby ruling out any diagrams that cannot be factorized in this sequential way. As in $\mathcal{H}^{\rm GNS}$, overcounting cannot occur.

A formal demonstration that Eq. (21) yields the same correlation structure as the standard formulation of parquet is not pursued here. What is already clear is that this proposal generates all self-consistent admixtures of the three permissible scattering arrangements for a many-particle system with a pair potential. The three core processes operate sequentially, never concurrently, in any combination generated from $\mathcal{H}^{\rm pqt}$.

For the reasons already noted for $\mathcal{H}^{\rm GNS}$ and illustrated in Fig. 8(b), intermediate particle-hole processes are not permitted within any particle-particle ladders for correlation diagrams derived from $\mathcal{H}^{\rm pqt}$. One would need to check that this did not restrict the parquet vertex structure [21,24–27] when interpreted, not as the diagrammatic architecture directly seen in the ground-state correlation energy but indeed as its functional derivative [4]; refer also to Eq. (A5) of Appendix A. Confirmation that Eq. (21) leads to standard parquet means reproducing the complete pair-scattering equations for this variationally generated dynamical vertex, to verify whether or not they are identical to their parquet analogs.

B. Induced interaction

The induced interaction [28,29] simplifies parquet by invoking a parametrized effective pair potential to stand in for the ladder sum of particle-particle scatterings. It has been effective as a theory of static properties in hard-core Fermi systems (nucleonic matter and noble-gas liquids) and their low-energy excitations as well [29]. A Coulomb-screened variant has been applied to the low-density electron gas [30].

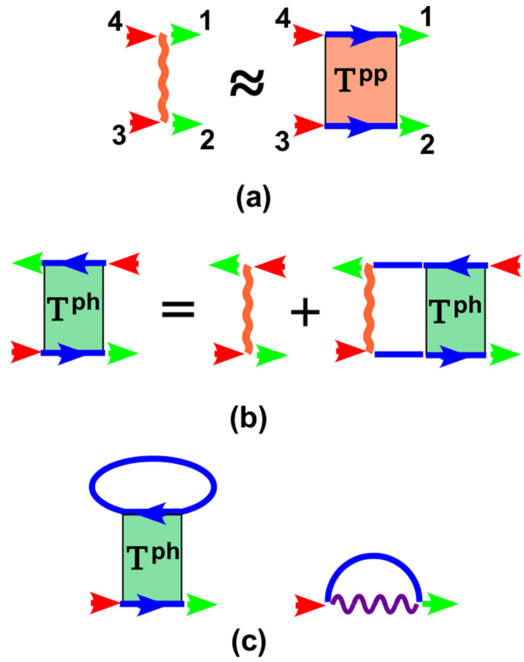

FIG. 9. Definition of the induced-interaction approximation. (a) The particle-particle T matrix, or ladder vertex, is replaced with an antisymmetrized effective potential $\overline{T}^{pp}$. (b) The particle-hole ladder series is defined by its Bethe-Salpeter equation; intermediate one-body propagators are self-consistently defined within the approximation as a whole. (c) The self-energy derived from the interaction Hamiltonian is determined by the particle-hole T matrix, selected via $\varphi^{(ph)}$, while the shielded interaction is selected through $\varphi^{(r)}$; the latter is defined as in Fig. 4(c) except that the bare potential V is replaced with the particle-particle ansatz $\overline{T}^{pp}$ schematized in (a) above.

In the induced interaction, explicit Brueckner-like particle-particle scattering is omitted. Instead, the bare potential $\langle k_1k_2|V|k_3k_4\rangle$ is replaced with an antisymmetrized approximation $\langle k_1k_2|\overline{T}^{pp}|k_3k_4\rangle$ to the ladders in Fig. 6(c); compare also Eq. (8). The Hamiltonian includes only ring and particle-hole processes manifestly:

$$\mathcal{H}^{\rm BB} = \sum_{\ell} \epsilon_k a_\ell^* a_\ell + \frac{1}{2N}\sum_{\ell_1\ell_2\ell_3\ell_4} \varphi^{\rm BB}_{\nu_1\nu_2|\nu_3\nu_4} \langle k_1k_2|\overline{T}^{pp}|k_3k_4\rangle a^*_{\ell_1} a^*_{\ell_2} a_{\ell_3} a_{\ell_4},$$

$$\varphi^{\rm BB}_{\nu_1\nu_2|\nu_3\nu_4} \equiv 1 - \left(1-\varphi^{(r)}_{\nu_1\nu_2|\nu_3\nu_4}\right)\left(1-\varphi^{(ph)}_{\nu_1\nu_2|\nu_3\nu_4}\right). \tag{22}$$

Figure 9 shows the essential ground-state correlation structure encoded in Eq. (22). Now we construct a pair of dynamical two-body scattering vertices, Γ for particle-hole and Ξ for ring processes (see Fig. 10), following the induced-interaction template [29,30]. Note that from now on a summation over an intermediate variable ℓ will be understood also to include intermediate integrals in the frequency domain subject to conservation as for momenta. In particular, the one-body causal propagator G_ℓ is now in frequency-dependent form [10].

The effective vertices Γ and Ξ subsume all noncanceling internal responses to an external disturbance. They include, but are not the same as, the vertex appearing in the equilibrium self-energy the induced-interaction form of which is shown in Fig. 9(c). Rather, they correspond to derived two-body scattering processes implicit in the correlation energy functional Φ but made manifest only through the dynamic response of the system [4]. Appendix A details the behavioral difference between the differently structured vertices.

The derived dynamical vertices should sum, consistently, all those intermediate two-body scatterings assured of surviving the internal stochastic averaging over $\varphi^{(ph)}$ and $\varphi^{(r)}$. Thus the Γ candidate is defined to have the structure

$$\Gamma(\ell_1\ell_2|\ell_3\ell_4) \equiv \langle k_1k_2|\overline{T}^{pp}|k_3k_4\rangle + \big(\varphi^{(ph)}_{\nu_1\nu_2|\nu_3\nu_4}\big)^{-1} \sum_{\ell'_1\ell'_2\ell'_3\ell'_4}{}' \Gamma(\ell_2\ell'_1|\ell_4\ell'_3)\varphi^{(ph)}_{\nu_2\nu'_1|\nu_4\nu'_3}\big(-\delta_{\ell'_1\ell'_4}\delta_{\ell'_2\ell'_3}G_{\ell'_1}G_{\ell'_2}\big)\varphi^{(ph)}_{\nu_1\nu'_2|\nu_3\nu'_4}\,\Xi(\ell_1\ell'_2|\ell_3\ell'_4)$$

$$= \langle k_1k_2|\overline{T}^{pp}|k_3k_4\rangle - \sum_{\ell}\Gamma(\ell_2\ell|\ell_4\ell')G_\ell G_{\ell'}\,\Xi(\ell_1\ell'|\ell_3\ell), \quad \ell' = \ell + \ell_3 - \ell_1. \tag{23}$$

This corresponds to the sum of "t-channel irreducible" processes [29], namely, those that cannot be separated into two subvertices by cutting any particle-hole line pair with momentum transfer $k_1 - k_3$. The negative sign in the summation on the right-hand side is due to exchange of one pair of particle (or hole) labels, relative to the complementary ringlike vertex Ξ; see Eq. (24) below. Any stochastic average with $\varphi^{(r)}$, for the object $\varphi^{(ph)}\Gamma$, will be suppressed owing to the vertex topology.

A concomitant summation gathers all ringlike scatterings defining Ξ, so

$$\Xi(\ell_1\ell_2|\ell_3\ell_4) \equiv \Gamma(\ell_1\ell_2|\ell_3\ell_4) + \big(\varphi^{(r)}_{\nu_1\nu_2|\nu_3\nu_4}\big)^{-1} \sum_{\ell'_1\ell'_2\ell'_3\ell'_4}{}' \Gamma(\ell_1\ell'_2|\ell'_3\ell_4)\varphi^{(r)}_{\nu_1\nu'_2|\nu'_3\nu_4}\big(\delta_{\ell'_1\ell'_3}\delta_{\ell'_2\ell'_4}G_{\ell'_1}G_{\ell'_2}\big)\varphi^{(r)}_{\nu'_1\nu_2|\nu_3\nu'_4}\,\Xi(\ell'_1\ell_2|\ell_3\ell'_4)$$

$$= \Gamma(\ell_1\ell_2|\ell_3\ell_4) + \sum_{\ell}\Gamma(\ell_1\ell''|\ell\ell_4)G_\ell G_{\ell''}\,\Xi(\ell\ell_2|\ell_3\ell''); \quad \ell'' = \ell + \ell_3 - \ell_2. \tag{24}$$

If we attempt an operation involving a stochastic average over $\varphi^{(ph)}$ of the RPA-like object $\varphi^{(r)}(\Xi - \Gamma)$, corresponding to the induced interaction's "u-channel irreducible" series (not separable into two subvertices by cutting any particle-hole line pair with momentum transfer $k_2 - k_3$), the result will be suppressed. Inspection of the series expansion of the latter shows that Eq. (24) has the symmetry

$$\Xi(\ell_1\ell_2|\ell_3\ell_4) = \Gamma(\ell_1\ell_2|\ell_3\ell_4) + \sum_{\ell}\Xi(\ell_1\ell''|\ell\ell_4)G_\ell G_{\ell''}\Gamma(\ell\ell_2|\ell_3\ell'').$$

Furthermore, substituting Γ from Eq. (23) into the right-hand side of Eq. (24) renders Ξ explicitly antisymmetric under pair exchange [29].

After averaging independently over the two stochastic restriction factors, the vertex Ξ emerging from Eqs. (23) and (24) leads to the set of dynamical two-body scattering processes within the induced-interaction model. As they stand, prior to any stochastic averaging, our vertex equations neglect all terms carrying the restriction factors $\varphi^{(r)}$ and $\varphi^{(ph)}$ concurrently. These remain legitimate parts of the complete Ξ, until the final average; when this is performed, the terms expressly left out of the coupled self-consistent pair Eqs. (23) and (24) are precisely those that vanish by destructive interference. Then Ξ becomes the induced-interaction vertex bearing the dynamic correlations in the model and determining its response functions, such as $\chi(\mathbf{q}, \omega)$, exhibited in Fig. 11.

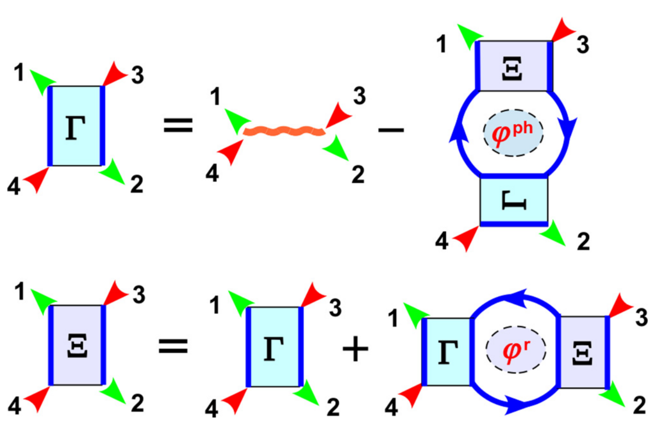

FIG. 10. Particle-hole and ringlike vertices mediate the dynamical interaction between particle and hole pairs in the induced-interaction model after its Hamiltonian, Eq. (22). These processes determine the system's self-consistent response to an external perturbation. The topology of the two-body vertex Γ sums all intermediate processes that are not automatically suppressed by stochastic averaging of its accompanying restriction factor $\varphi^{(ph)}$. Correspondingly, the interaction vertex Ξ includes all possible topologies that are not automatically suppressed by an average over the rings-only factor $\varphi^{(r)}$. Also note that the phenomenological particle-particle vertex $\overline{T}^{pp}$ is antisymmetrized for particle-pair exchange $1 \leftrightarrow 2$ or $3 \leftrightarrow 4$. Thus the complete induced-interaction scattering amplitude Ξ is itself antisymmetric.

VI. SUMMARY

The goal of this paper has been the rational construction of explicit Hamiltonians for significant conserving approximations lacking them, in problems of strongly interacting

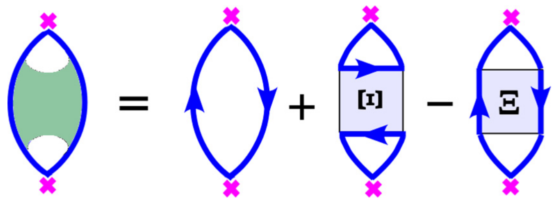

FIG. 11. Total density-density response function determined by the self-consistent two-body vertex structure in the induced-interaction model. Crosses indicate coupling to a weak external perturbing potential. (If coupling is to the current, its operator attaches to the external vertices and the diagram describes the current autocorrelation function.) The leading right-hand term is the renormalized polarization with no particle-hole vertex; the second incorporates the contributions generalizing Hartree-like (RPA) screening; the last term holds the complementary particle-hole ladders responsible for Fock-like exchange scattering.

assemblies. Chief among the many-body problems of interest are short-range dynamics in charged quantum fluids such as the electron gas, as well as nuclear matter and the noble-gas fluids.

Conventionally, diagrammatic theories of correlations have been set up via other microscopic prescriptions, such as Φ derivability, but methods that build their correlation structure heuristically from the bottom, so to speak, do not generate a Hamiltonian corresponding to their model. This can make it problematic to confirm essential canonical properties, notably the conserving sum rules, which are hallmarks of the exact theory and which one wants to validate equally for any approximate description.

A systematic strategy for constructing model Hamiltonians was formulated by Kraichnan. It consists in (i) embedding the exact interacting problem within a large ensemble of identical but distinguishable system copies, (ii) adjoining, to their exact interaction potential, randomly chosen factors coupling stochastically all the copies in the collection, and (iii) designing the coupling scheme so that only specific restricted sets of expectation values for correlations will survive stochastic averaging over the introduced couplings. All other combinations will be suppressed by destructive interference and vanish in the limit of an infinite ensemble average.

Correlations selected in that way will bring out the effects believed to prevail in a given physical context. For example, one form of stochastic coupling will pick out screening correlations in a characteristically long-ranged Coulomb system. Another form will promote repeated particle-particle scattering in systems with a hard-core potential.

First, the technicalities of Kraichnan's construction were recalled. Next came a survey of applications originally given by Kraichnan. Included were the random-phase and Hartree-Fock approximations and their refinement in the shielded potential, or ring, model, and the ladder series for hard-core systems such as nuclear matter. These steps set the scene for the third part: adaptation of the stochastic method to more elaborate correlation theories for which a Hamiltonian has not been at hand.

Three approximations of interest were discussed and Hamiltonians were identified for them. All involve a microscopically consistent unification of short-range with long-range correlations. They are the ring-plus-ladder model, the parquet theory, and the induced-interaction construction. For the latter an explicit pair of particle-hole dynamical scattering-vertex equations was described, based on a generalized definition of the stochastic coupling factor. I showed that the vertex equations definable within the stochastic Hamiltonian formalism are the same as their heuristic counterparts establishing the induced interaction.

Appendix A examines the role and interpretation of the sum rules in conserving models, concentrating on the third frequency-moment sum rule. The sum-rule structure for a conserving approximation follows canonically from its Hamiltonian (when known) inheriting its analytic properties from the complete system description. However, care has to be taken with how these relations are evaluated and interpreted. Other identities that are not sum rules and valid for the exact system need not hold in an approximation [33], the price of any simplification. Still, an advantage of knowing the Hamiltonian is automatic validity for all sum rules that come out of microscopic conservation plus the causal boundary conditions. One has only to apply the rules discerningly. Appendix B contains brief remarks on possible relations between the existence of approximate interacting Hamiltonians and complementary nondiagrammatic solutions to general correlation problems.

Future work would include a demonstration that the proposed parquet Hamiltonian Eq. (21) yields a dynamical two-body vertex structure identical to that originally worked out in the parquet literature. To the extent that parquet in particular has an intimate link to nonperturbative variational methods in strong correlations [21,25], any consequences of confirming the parquet Hamiltonian follow through for those approaches. At a more general level, as sketched in Appendix B, similar considerations might be applied to any interacting model reliant on an underlying Hamiltonian. One could also explore how Kraichnan's stochastic Hamiltonians may apply with increasing sophistication and physical fidelity beyond linear response and in lower dimensions [14,34], not only in uniform Coulomb systems but in inhomogeneous interacting systems of all types. As a conceptual tool, some of its power may have been demonstrated in this paper. As a practical tool it awaits further thought.

ACKNOWLEDGMENTS

I thank Prof. Kenneth Golden for stimulating my return to this long-standing problem, Prof. Mukunda Das for his forthright and invariably fruitful comments as the work developed, and Prof. Alexander Lande for directing me to Ref. [27] and its extension of the parquet approach to three-body correlations.

APPENDIX A: THIRD FREQUENCY-MOMENT SUM RULE

The importance of the third frequency-moment sum rule for short-range correlation properties, Coulomb fluids included, was first highlighted by Goodman and Sjølander [35]. They gave a proof of the rule and analyzed the information it contains about the near environment, or "correlation hole," of a typical particle within its interacting medium.

Here we focus upon the relevance of this sum rule as a paradigm for the way in which approximate correlation models, despite being assured of satisfying the sum rules of the full case, call for a more careful understanding of what the sum rules may have to tell. We will not detail the proof of the third-moment rule, relying on Ref. [35]; a more diagrammatically oriented proof is in Ref. [16].

We state the rule as it applies to the electron fluid. If one takes the dynamic and static structure factors for the system [2,35], respectively $S(q,\omega)$ and $S(q)$, the third-moment rule is

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\omega^3 S(q,\omega) = \frac{q^4 n}{2}M_3(q),$$
$$M_3(q) \equiv \frac{q^2}{4} + 2\sum_k \varepsilon_k\langle a_k^* a_k\rangle + V(q)n\left\{1 - n^{-1}\sum_{q'}(\hat{\mathbf{q}}\cdot\hat{\mathbf{q}}')^2[S(q') - S(|\mathbf{q}-\mathbf{q}'|)]\right\}. \tag{A1}$$

Unlike the first-moment (f-sum) rule, this identity gives weight to the high-frequency (short-time, thus also short-ranged) properties of the assembly. Hence it is much more sensitive to the correlation structure. That is evident through the second right-hand term of the factor $M_3(q)$, which is the expectation of the kinetic energy over the interacting Fermi sea. Sensitivity to correlations comes out even more clearly in the last contribution, explicitly dependent on the static structure factor the nature of which we now discuss.

In addressing the structure factor $S(q)$ we make an important observation. Through its manifest sensitivity to the correlations in the system, Eq. (A1) for the third-moment rule will equally reflect the correlation properties of any approximation to the exact physics. By that it may also accentuate the physical shortcomings of the approximation, so the rule is an important quantitative gauge of a model. The latter does not touch the architecture of the rule, which remains valid; it means that one must be careful how the right- and left-hand sides of Eq. (A1) have to be evaluated.

Commonly termed the "static" structure factor, $S(q)$ is the instantaneous pair-correlation function in Fourier space:

$$S(q) \equiv \sum_{kk'}\langle a_{k+q}^* a_k a_{k'-q}^* a_{k'}\rangle. \tag{A2}$$

Mathematically it is generated by direct removal of an interaction line in the diagrammatic expansion for Φ:

$$S(q) \equiv \frac{\delta\Phi}{\delta V(-q)}; \tag{A3}$$

its inner structure therefore represents the equilibrium correlation structure directly [16]. By contrast, the dynamic structure factor is the density response to a weak, but external, perturbation itself coupling to the density. This is in sharp functional distinction to $S(q)$, which is strictly determined in the ground state. We stress that $S(q,\omega)$ is not an equilibrium property although it is computed in terms of equilibrium expectation values.

Now we look at how Φ is perturbed. A weak external potential U couples to the density operator through a one-body term $U(q,\omega)a_{k+q}^* a_k$ added to the Hamiltonian, Eq. (1). This changes the correlation energy:

$$\Phi[U] = \Phi[0] + \tfrac{1}{2}U^*(q,\omega)\chi(q,\omega)U(q,\omega) + \mathcal{O}(|U|^4); \tag{A4}$$

there is no linear term since Φ is a minimum at equilibrium. However, obtaining the response function is no longer a simple matter of removing an interaction line from Φ, as for $S(q)$. We must track down every occurrence of U including its appearance in the self-consistently recurrent structure of the propagators $G[U]$. A clear and very detailed exposition of the process is in Refs. [4,5].

Let $\Lambda[G]$ be the vertex defining the correlation energy so that, symbolically, the perturbed self-energy is $\Sigma \equiv U^* + \Lambda[G]{:}G[U]$ where for brevity we denote by ":" internal integrations over momentum energy. The dynamic response to lowest order in the perturbation is encoded in the quantity

$$\begin{aligned}\delta\Phi &= \frac{1}{2}U^*:\left[\frac{\delta G}{\delta U} + \frac{\delta G}{\delta U^*}:\frac{\delta^2\Phi}{\delta G\delta G'}:\frac{\delta G'}{\delta U}\right]:U\\ &= \frac{1}{2}U^*:\left[\frac{\delta G}{\delta U} + \frac{\delta G}{\delta U^*}:\Lambda:\frac{\delta G'}{\delta U}\right.\\ &\quad\left.+\left(\frac{\delta G}{\delta U^*}:\frac{\delta\Lambda}{\delta G''}:\frac{\delta G''}{\delta U}:G' + G:\frac{\delta G''}{\delta U^*}:\frac{\delta\Lambda}{\delta G''}:\frac{\delta G'}{\delta U}\right)\right]:U.\end{aligned} \tag{A5}$$

Aside from the leading term $\delta G/\delta U = GG$ on the right-hand side of the second expression (the renormalized zeroth-order polarization), comparison of Eqs. (A4) and (A5) shows that the diagrammatic structure of the dynamic response $\chi(q,\omega)$ is not solely determined by that of Λ, the terms of which appear in the ground-state energy functional directly defining the conserving one-body $\Sigma[G]$, but also, and crucially for microscopic conservation at the two-body level, by the new contributions generated through self-consistency of the correlations in the system [4,31]. The phenomenon is illustrated in Figs. 4(b), 6(b) and 7(b) for the three primary models of Sec. III and in Fig. 11 for Sec. V.

The central message of this discussion is that, for any description of a correlated system, $S(q,\omega)$ as the negative imaginary part of $\chi(q,\omega)$ has explicit extra terms appearing in it that are otherwise dormant in the ground-state energy functional. In any approximate picture of correlations, in other words, the dynamical vertex and its $S(q,\omega)$ on the one hand will not have the same diagrammatic structure as the ground state and its $S(q)$ on the other.

These objects lead to quite different results. This does not contradict the fact that all the sum rules that apply to the full theory—including the correlation-sensitive third-moment rule—remain valid in any approximation built on the Kraichnan or functionally equivalent Φ-derivable pattern. It comes down to a consistent reading of the sum rules.

Equation (A1) in any approximate model is interpreted correctly if, and only if, the dynamic structure factor on the left-hand side derives from Eq. (A5) while, on the right-hand side, the static structure factor is obtained from Eq. (A3). That is because, in diagrammatic terms, the prime physical basis of $S(q)$ resides directly in the ground-state properties through Λ [16]; true in the exact case, it is thus true for any properly constituted approximation.

Confusion has sometimes arisen over this conceptual point, not just for the third-moment sum rule but for other instances such as the compressibility sum rule [36]. In the exact theory—and in the exact theory alone—the static factor $S(q)$ has another, possibly more familiar, expression as the frequency integral of $S(q,\omega)$ [2]:

$$S(q) = \int_0^\infty d\omega S(q,\omega). \tag{A6}$$

In experiment this relation gives the scattering cross section from an angle-resolved measurement uncollimated for inelastic energy loss ω, the cross section of which as measured would be $S(q,\omega)$. Interpreted theoretically, its strongly model-dependent form is not a sum-rule identity obtained from standard arguments using analyticity and the Kramers-Krönig relations [11], the causal structure of which is immune to ensemble averaging.

If applied in any *approximation* to the full problem, Eq. (A6) fails to yield the same result as Eq. (A3). For the RPA, Eq. (A3) results in a trivial pair-correlation function in real space with no features at all, while Eq. (A6) for RPA results in a pair-correlation function that becomes unphysically negative [11]. Thus, by itself, formal conservation hardly secures good numbers in a model, but feeding the evaluation of Eq. (A6) into the right-hand side of Eq. (A1) makes matters worse by breaking sum-rule consistency.

Suppose we had obtained, from Eq. (A3), a poor estimate for $S(q)$ compared to measurement. We might turn to Eq. (A6), somewhat unsystematically in this context, expecting a better answer (with no guarantee of improvement). Unfortunately this forfeits its canonical pedigree from the model Hamiltonian because the third-moment sum rule would be violated with that choice.

As far as is known the equivalence of (A3) and (A6) is only for the exact ground state [33]. The reason appears to be the dependence of Eq. (A6) on Fermi's "golden rule" [2], itself exploiting completeness of the many-body eigenstates in Fock space. In the Kraichnan ensemble average, the contribution of whole families of states is washed out (albeit, prior to averaging, the completeness of Fock space holds for each individual member in the ensemble of stochastic Hamiltonians). This kills the state coherence essential to Eq. (A6).

It is reasonable to surmise that the distinction between a set of virtual (dormant) dynamic correlations in $S(q)$ and their real manifestation in $S(q,\omega)$, mandated by conservation [4], applies to the actual exact description. Then Eq. (A6) reveals a deeper and extremely rigid constraint on the terms beyond those in Λ on the right-hand side of Eq. (A5), impossible to meet within any approximation [33]. The discrepancy between the two evaluations of $S(q)$, canonical for Eq. (A3) but in practice empirical for (A6), is the price paid by any truncation of the full problem, no matter how elaborate. Indeed, it could be used as an in-built measure of the mismatch between a reduced correlation theory and its fully correlated parent.

APPENDIX B: KRAICHNAN'S CONSTRUCTION AND NONDIAGRAMMATIC ANALYSES

This Appendix remarks informally on how the stochastic-Hamiltonian approach may relate to self-consistent correlated theories not reliant on diagrammatic analysis characteristic of Green-function methodology. We focus on two nonperturbative examples: density-functional theory [17,18] and the coupled-cluster formalism [19,20].

1. Density-functional theory

Basic to density-functional theory (DFT) is the proof that the ground-state energy expectation of a many-body system interacting in the normal state is a unique functional of its particle-density distribution [17]. Then, given an independent constitutive relation between particle density and exchange-correlation energy density, the problem of determining the interacting system's behavior can be closed and solved.

There are many ways to negotiate approximate closures for DFT, but the *exact* formulation of its basic Hohenberg-Kohn and Kohn-Sham theorems [17] is not negotiable. The question arises whether there exist physically meaningful approximations to correlated systems for which the foundational DFT theorems are equally valid. That indeed there are such models was established by Langreth [18].

In brief, Langreth demonstrates that any Φ-derivable correlation model (its exchange-correlation energy functional meets the Baym-Kadanoff criteria for microscopic conservation [4,5]) will satisfy the DFT theorems. Hence any method for solving the DFT equations is applicable to this wide class of model. These offer a different quality and order of approximation over and above strategies such as local-density and generalized-gradient methods [17], ordinarily invoked to solve density-functional problems.

Our present paper has shown how extended models of correlations based on Kraichnan's Hamiltonian structures are equivalent to the Φ-derivable description of their free-energy functional. From Ref. [18] it follows that there are physically nontrivial density-functional theories that, while approximate, possess a fully defined and valid Hamiltonian in the sense of Kraichnan. Any useful implications for DFT praxis fall outside our ambit here and would need closer study within that specific context.

2. Coupled-cluster method

The situation of the coupled-cluster method (CCM) (also known as "exp S") [19,20], vis à vis the existence of model Hamiltonians, at first glance is not dissimilar to the case of DFT. One way to make a connection is to note that the coupled equations defining the exp S method [19] address certain overlap integrals for the Hamiltonian, selecting the set of "linked" amplitudes that determine the irreducible contributions to the correlation-energy functional $\Phi[V]$, already discussed in Sec. IV.

If one embeds the Hamiltonian of the CCM using the Kraichnan prescription for its interaction part Eq. (6), along with a physically guided choice for the restriction parameters $\varphi_{\nu_1\nu_2|\nu_3\nu_4}$, then an appropriate coupled-cluster formulation exists *for each member of the Kraichnan ensemble* as well as collectively. Subsequently this assembly would be subject to stochastic averaging just as in the diagrammatic approach. One would need to ask how the exp S equations changed in any process of reduction and, importantly, whether the operation of taking overlap integrals in exp S should be expected to commute with that of stochastic averaging, for the same distinction seen in Appendix A would arise between canonical procedures immune to stochastics and those sensitive to the accompanying loss of state completeness.

Answers to these issues may lie in the fact that the (nondiagrammatic) coupled-cluster formalism has a correspondence to the (diagrammatic) Goldstone time-ordered expansion [19] and therefore in principle has a path back to Φ derivability [5]. Further investigations along such lines would be enlightening.

A different aspect of CCM is its hierarchical truncation of linked amplitudes ("SUB2", "SUB3," etc., within the terminology). It is difficult to tell—at this point—whether suitable Kraichnan restriction parameters φ could be systematically defined for these. A possible analogy is the treatment of RPA and Hartree-Fock within the Kraichnan approach (see Secs. III A and III B) where truncation via their corresponding φ is not stochastic at all, but simply sets to zero anything beyond those two basic correlations. Even diagrammatically it is an open question whether something equally prescriptive and not stochastic operates at higher orders of correlation. It suggests a very interesting problem that could also, in its turn, shed light on the nature of Kraichnan's program itself.

[1] D. Pines and D. Bohm, Phys. Rev. **85**, 338 (1952).
[2] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966).
[3] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).
[4] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961).
[5] G. Baym, Phys. Rev. **127**, 1391 (1962).
[6] A. A. Abrikosov, L. P. Gor'kov, and I. Ye. Dzyaloshinskii *Quantum Field Theoretical Methods in Statistical Physics*, 2nd ed. (Pergamon, Oxford, 1965).
[7] L. V. Keldysh, Zh. Eksp. Teor. Fiz. **47**, 1515 (1964); translation: Sov. Phys. JETP **20**, 1018 (1965).
[8] D. C. Langreth, *Linear and Nonlinear Electron Transport in Solids*, NATO Advanced Studies Series, edited by J. T. Devreese and V. E. van Doren (Plenum, New York, 1976), pp. 3–32.
[9] P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1964).
[10] G. Rickayzen, *Green Functions and Condensed Matter* (Academic, London, 1980).
[11] G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
[12] P. Coleman, *Introduction to Many-Body Physics* (Cambridge University, Cambridge, England, 2015).
[13] R. H. Kraichnan, J. Math. Phys. **3**, 475 (1962).
[14] R. H. Kraichnan, J. Math. Phys. **3**, 496 (1962).
[15] S. Chen, G. Eyink, G. Falkovich, U. Frisch, S. Orszag, and K. Sreenivasan, Phys. Today **61**, 70 (2008).
[16] F. Green, D. Neilson, D. Pines, and J. Szymański, Phys. Rev. B **35**, 133 (1987).
[17] *Electronic Density Functional Theory: Recent Progress and New Directions*, edited by J. F. Dobson, G. Vignale, and M. P. Das (Plenum, New York, 1998).
[18] D. C. Langreth, Phys. Rev. Lett. **52**, 2317 (1984).
[19] H. Kümmel, K. H. Lührmann, and J. G. Zabolitzky, Phys. Rep. **36**, 1 (1978).
[20] J. S. Arponen, R. F. Bishop, and E. Pajanne, Phys. Rev. A **36**, 2519 (1987); **36**, 2539 (1987).
[21] A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982).
[22] F. Green, D. Neilson, and J. Szymański, Phys. Rev. B **31**, 2779 (1985).
[23] F. Green, D. Neilson, and J. Szymański, Phys. Rev. B **31**, 2796 (1985).
[24] R. W. Haymaker and R. Blankenbecler, Phys. Rev. **171**, 1581 (1968).
[25] A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rev. Lett. **54**, 1469 (1985).
[26] A. Lande and R. A. Smith, Phys. Lett. B **131**, 253 (1982).
[27] A. Lande and R. A. Smith, Phys. Rev. A **45**, 913 (1992).
[28] S. Babu and G. E. Brown, Ann. Phys **78**, 1 (1973).
[29] T. L. Ainsworth and K. S. Bedell, Phys. Rev. B **35**, 8425 (1987).
[30] T. L. Ainsworth, F. Green, and D. Pines, Phys. Rev. B **42**, 9978 (1990).
[31] D. F. DuBois and M. G. Kivelson, Phys. Rev. **186**, 409 (1969).
[32] K. A. Brueckner and J. H. Gammel, Phys. Rev. **109**, 1023 (1958).
[33] A. D. Jackson and R. A. Smith, Phys. Rev. A **36**, 2517 (1987).
[34] W. Magnus and W. Schoenmaker, *Quantum Transport in Submicron Devices* (Springer, Berlin, 2002).
[35] B. Goodman and A. Sjølander, Phys. Rev. B **8**, 200 (1973).
[36] P. Vashishta and K. S. Singwi, Phys. Rev. B **6**, 875 (1972).