Hamiltonian perspective on parquet theory

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Understanding collective phenomena calls for tractable descriptions of correlations in assemblies of strongly interacting constituents. Capturing the essence of their self-consistency is central. The parquet theory admits a maximum level of self-consistency for strictly pairwise many-body correlations. While perturbatively based, the core of parquet and allied models is a set of strongly coupled nonlinear integral equations for all-order scattering; tightly constrained by crossing symmetry, they are nevertheless heuristic. Within a formalism due to Kraichnan, we present a Hamiltonian analysis of fermionic parquet's structure. The shape of its constitutive equations follows naturally from the resulting canonical description. We discuss the affinity between the derived conserving scattering amplitude and that of standard parquet. Whereas the Hamiltonian-derived model amplitude is microscopically conserving, it cannot preserve manifest crossing symmetry. The parquet amplitude and its refinements preserve crossing symmetry, yet cannot safeguard conservation at any stage. Which amplitude should be used depends on physics rather than on theoretically ideal completeness.

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I. INTRODUCTION

In this paper we explore a canonical basis for a significant class of theories of many-particle correlations. Growth in computing capacity has fueled increasingly comprehensive studies of assemblies of interacting elements and how these come to determine the behavioral complexity of such assemblies, at simulational and analytical levels. The resulting numerics feed back to expand theoretical concepts of how a system's elementary components, with their interactions, cooperate in subtle collective phenomena.

Among long-established formulations are the conserving Φ-derivable approximations after Kadanoff and Baym [1,2] and an especially significant candidate, parquet theory [3–6]. Our program also covers parquetlike variants such as the induced interaction [7–9] which has a successful record in its own right for problems of strong correlations. There is conceptual merit in codifying the intuition behind these heuristic models in a more top-down way.

Φ derivability concerns the response structure that emerges from constructing, as its generator, an effective correlation energy functional Φ. In parquet one constructs the correlated two-body scattering amplitude directly. The interrelationship of parquet and Φ derivability has been analyzed previously [10–13] though not from a Hamiltonian point of view.

Parquet, its relatives, and the Φ-derivable descriptions are all constructed by choosing judiciously, if by hand, physically dominant substructures out of the complete set of correlation energy diagrams. Parquet theory stands out by including topologically the largest conceivable set of particle-particle-only and particle-hole-only pair scattering processes. This maximally pair-coupled topology makes it worth seeking canonical grounds for parquet to shed a different light on its structure.

Emerging from a formalism relatively unfamiliar to many-body practice, our conclusions turn out to resonate strongly with the diagrammatic investigation by Smith [11]. To establish a Hamiltonian basis for the class of theories in question, we adapt the strategy originally devised by Kraichnan [14,15] and applied recently to a series of simpler self-consistent diagrammatic models [16]. These are Φ derivable in the sense of Baym and Kadanoff; they each possess a model Luttinger-Ward-like correlation energy functional [17] as the generator of static and dynamic response and correlation functions which, while approximate, strictly conserve particle number, momentum, and energy at both microscopic and global levels.

In essential form the parquet scattering amplitude is subsumed under a specific Φ-derivable description, the fluctuation-exchange (FLEX) approximation [6]. Although considered incomplete and subject to refinement, the simplest configuration of parquet is thus already a component of a correlated model whose desirable microscopic conservation properties follow naturally. What is not in place is a Hamiltonian underpinning for FLEX.

To arrive at any conserving response formulation a price is paid in committing to a canonical Hamiltonian description. Granted all its consequent analytical benefits, there is a caveat on the possibility of further consistent refinement of parquet beyond its basic form emerging directly from FLEX: diagrammatic iteration of the renormalized two-body parquet amplitude, feeding it back into the one-body self-energy functional, cannot achieve control over conservation [11]. We revisit this in the following.

Kraichnan's embedding of the many-body problem in a larger space departs substantially from traditional diagrammatic reasoning. It is central to the project because it is applicable to systems with pair interactions. In principle it should have something to say about parquet.

One starts by injecting the physical Hamiltonian into a much larger sum (going to infinity) of identical but distinguishable replicas. A collective representation is introduced over this total Hamiltonian. Next, isomorphic copies of these large collective Hamiltonians are themselves summed into a grand Hamiltonian, but with the interaction potential of each collective copy now partnered by an individual coupling factor. The factor depends only on the collective indices as V depends only on the physical indices. Adjoined to V in this way, the coupling can be defined stochastically.

Provided the couplings transform in their abstract indices as the elementary pair potential transforms in its physical indices, the end result is a Hamiltonian in which the original physical form is embedded. Left unmodified, with all coupling factors set to unity, the expanded system recovers the exact physics. If modified appropriately, all the unitary properties of the collective Hamiltonians, and of their grand sum, are unaffected.

Contingent upon the functional form of the couplings, any operator expectation over their distribution in the superassembly allows subsets of the exact correlation-energy diagrams at any order to survive when their overall coupling-factor product works out as unity, thus imparting immunity to taking the expectation. All other products of random coupling factors are asymptotically killed off by mutually destructive interference in the expectation: an extension of the random-phase approximation [18].

The key to the strategy is that, up to averaging over Kraichnan's couplings, the superensemble represents a well-defined many-body Hamiltonian. Each collective member is distinguished by its own assignment of coupling factors and corresponds to a precisely defined Fock space. This means that any exact identity in the hierarchy of analytic Green functions will survive averaging if (and only if) the averaging process is done consistently on both sides of the relation. This covers the Ward-Pitaevsky identities between one-body self-energy and two-body response kernel, and Kramers-Krönig analyticity leading to the frequency sum rules for the correlation functions [19]. Relations that do not rely on analyticity are not preserved, however. We clarify the distinction in the following.

One is therefore justified in discussing a canonical Hamiltonian for the diagrammatic approximation giving the expectation for Φ over the distribution of Kraichnan's coupling factors. To cite Baym [2]: "One reason underlying the fact that these approximations have such a remarkable structure has been discovered by Kraichnan, who has shown that in a certain sense they are exact solutions to model Hamiltonians containing an infinite number of stochastic parameters."

Unlike in a physically guided, constructive Φ-derivable model, the approximation is encoded here *a priori* in the couplings of the Kraichnan Hamiltonian. This does not mean "from first principles," as the intuitive task of isolating dominant terms is merely shifted from the choice of a diagram subset for Φ to that of an appropriate Kraichnan coupling (K coupling hereafter). It really means that classes of conserving consistency properties, though not all, that are fundamental in the canonical description hold automatically after averaging.

Section II starts with a minimal review of Φ derivability, recalling properties essential in building up a conserving many-body expansion. Kraichnan's formalism [14–16] is then introduced and a form of it proposed, including all possible pairwise-only interactions. In Sec. III we revisit the logical development of the pairwise correlation structure of the Kraichnan model's response to a perturbation. This teases out real physical effects otherwise dormant, or virtual, in the self-consistent structure of Φ itself. Finally in Sec. IV we arrive at the parquet equations' scaffold, displaying its provenance from the Hamiltonian defined after Kraichnan. There too we discuss conceptual points of difference between parquet topology interpreted within the Hamiltonian outlook, and attempts to enlarge the topology by an iterative feedback; these do not accord with Φ derivability.

Despite their affinity, Φ derivability and parquet analysis exhibit complementary inherent shortcomings deeply linked to the general nature of so-called planar diagrammatic expansions [10,11]. This invites care in considering which sets of physical problems are better served by one or the other of the two approaches. We offer concluding observations in Sec. V.

II. PRECISE HAMILTONIANS FOR APPROXIMATE MODELS

A. Correlation energy

Our many-body system has the second-quantized Hamiltonian

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

in terms of one-particle creation operators a^* and annihilation operators a. The first right-hand term is the usual total kinetic energy; the second term is the pairwise interaction. For simplicity we discuss a spin- (or isospin-)independent scalar V but this can be relaxed without invalidating the argument for pair interactions. Here, again for simplicity, we address a spatially uniform system for which momentum is a good quantum number; index k stands for the wave vector and spin pair $(\mathbf{k}, s)$, writing a_k^* as the creation operator with a_k the annihilation operator, both satisfying fermion anticommutation. The summation $\sum'_{k_1k_2k_3k_4}$ comes with the restriction $k_1 + k_2 = k_3 + k_4$. In a neutral uniform Coulomb system, potential terms with $k_2 - k_3 = 0 = k_4 - k_1$ are canceled by the background and are excluded.

The ground-state energy resulting from the full Hamiltonian includes a correlation component $\Phi[V]$, the essential generator for the diagrammatic expansions that act as vocabulary to the grammar of the analysis. Here we go directly to $\Phi[V]$ and for full discussion of the interacting ground-state structure we refer to the classic literature [2,17]. The correlation energy can be written as a coupling-constant integral

$$\Phi[V] \equiv \frac{1}{2}\int_0^1 \frac{dZ}{Z} G[ZV] : \Lambda[ZV; G] : G[ZV] \tag{2}$$

in which $G[V]$ is the complete renormalized two-point Green function of the system, describing propagation of a single particle in the presence of all the rest, and $\Lambda[V; G]$ is the fully renormalized four-point scattering amplitude whose internal structure manifests all the possible modes by which the propagating particles (via G) interact via V. Single dots "$\cdot$" and double dots ":" denote single and double internal integrations, respectively, over frequency, spin, and wave vector, rendering $G : \Lambda : G$ an energy expectation value.

The renormalized Green function satisfies Dyson's equation

$$G[V] = G^{(0)} + G^{(0)} \cdot \Sigma[V; G] \cdot G[V] \tag{3}$$

with $G^{(0)}$ as the noninteracting Green function $G_k^{(0)}(\omega) \equiv (\omega - \varepsilon_k)^{-1}$ with $\Sigma[V; G]$ as the self-energy. Equation (3) links back to the correlation-energy functional self-consistently through the variation that defines the self-energy:

$$\Sigma[V; G] \equiv \frac{\delta\Phi[V]}{\delta G[V]} = \Lambda[V; G] : G[V]. \tag{4}$$

We recall the basic requirements on Λ. In the expansion to order n in V within any particular linked structure of $G : \Lambda[V; G] : G$ reduced to its bare elements, there will be $2n$ bare propagators. The integral effectively treats each $G^{(0)}$ as distinguishable, and there is a $2n$-fold ambiguity as to which bare propagator should be the seed on which the given contribution is built. That is, integration replicates the same graph $2n$ times from any particular $G^{(0)}$ in the integral, but the structure contributes once only in Φ. The coupling-constant formula removes the multiplicity to all orders.

The essential feature of Λ in the exact correlation energy functional is the following symmetry: consider the skeleton $G^{(0)} : \Lambda[V; G^{(0)}] : G^{(0)}$. Removal of any $G^{(0)}$ from the skeleton, *at any order in* V, must result in the same unique variational structure; all lines are equivalent. The same applies when all bare lines are replaced with dressed ones [1]. This is due to unitarity and ultimately to the Hermitian character of the Hamiltonian. It also follows that Λ must be pairwise irreducible: removing any two propagators G from $G : \Lambda : G$ cannot produce two unlinked self-energy insertions, or else there would be inequivalent Gs in a contribution of form $G : \Lambda_1 : GG : \Lambda_2 : G$. These conditions impose a strongly restrictive graphical structure upon the four-point scattering kernel entering into the self-energy.

B. Φ derivability

Other than the generic symmetry of G in Φ, the variational relationships among Λ, Σ, and G do not depend on topological specifics. Those relationships were thus adopted as defining criteria by Baym and Kadanoff [1,2] for constructing conserving approximations: the Φ-derivable models. Choosing a subset of skeleton diagrams from the full $\Phi[V]$ with every $G^{(0)}$ topologically equivalent and replacing these with dressed lines guarantees unitarity of the effective model Λ and secures microscopic conservation not only at the one-body level but also for the pairwise dynamic particle-hole response under an external perturbation.

Φ derivability necessarily entails an infinite-order approximation to the correlation structure in terms of the bare potential. While a finite choice of skeleton diagrams of Φ fulfills formal conservation, it must still lead to an infinite nesting of bare interactions linked by pairs of renormalized Gs. Self-consistency in Eqs. (3) and (4) is a fundamental feature of all Φ-derivable models.

C. Kraichnan Hamiltonian

The authoritative references for Kraichnan Hamiltonians are the original papers of Kraichnan [14,15]. Here we follow the more recent paper by one of us, hereafter called KI [16]. As per the Introduction, Kraichnan's construction proceeds by two ensemble-building steps. First, one generates an assembly of N functionally identical distinguishable copies of the exact Hamiltonian, Eq. (1). The total Hamiltonian is

$$\mathcal{H}_N = \sum_{n=1}^{N} \sum_k \varepsilon_k a_k^{*(n)} a_k^{(n)} + \frac{1}{2} \sum_{n=1}^{N} \sum_{k_1 k_2 k_3 k_4} \langle k_1 k_2 | V | k_3 k_4 \rangle \, a_{k_1}^{*(n)} a_{k_2}^{*(n)} a_{k_3}^{(n)} a_{k_4}^{(n)}. \tag{5}$$

The creation and annihilation operators with equal index n anticommute as normal; for values of n that differ, they commute. At this point one goes over to a collective description of the N-fold ensemble by Fourier transforming over index n. For integer ν define the collective operators

$$a_k^{*[\nu]} \equiv N^{-1/2} \sum_{n=1}^{N} e^{2\pi i \nu n/N} a_k^{*(n)} \text{ and } a_k^{[\nu]} \equiv N^{-1/2} \sum_{n=1}^{N} e^{-2\pi i \nu n/N} a_k^{(n)}. \tag{6}$$

These preserve anticommutation up to a term strongly suppressed by mutual interference among unequal phase factors and at most of vanishing order $1/N$. The argument is a random-phase one [18]:

$$\begin{aligned}
\left[a_k^{*[\nu]}, a_{k'}^{[\nu']}\right]_+ &= \frac{1}{N} \sum_{n,n'} e^{2\pi i(\nu n - \nu' n')/N} \left[a_k^{*(n)}, a_{k'}^{(n')}\right]_+ \\
&= \frac{1}{N} \sum_{n} e^{2\pi i(\nu - \nu')n/N} \left[a_k^{*(n)}, a_{k'}^{(n)}\right]_+ + \frac{2}{N} \sum_{n \neq n'} e^{2\pi i(\nu n - \nu' n')/N} a_k^{*(n)} a_{k'}^{(n')} \\
&= \delta_{kk'} \delta_{\nu\nu'} + O(N^{-1}),
\end{aligned} \tag{7}$$

and similarly for $[a_k^{[\nu]}, a_{k'}^{[\nu']}]_+$. In practice, any term in the Wick expansion of physical expectations that links dissimilar elements $n \neq n'$ will not contribute in any case. The transformation yields the new representation

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

$$\equiv \sum_\ell \varepsilon_k a_\ell^* a_\ell + \frac{1}{2N} \sum_{\ell_1 \ell_2 \ell_3 \ell_4}{}' \langle k_1 k_2 | V | k_3 k_4 \rangle \, a_{\ell_1}^* a_{\ell_2}^* a_{\ell_3} a_{\ell_4}, \tag{8}$$

where in the last right-hand expression we condense the notation so $\ell \equiv (k, \nu)$ and the restriction on the sum now comprises $\nu_1 + \nu_2 = \nu_3 + \nu_4$ (modulo N) as well as the constraint on the momenta; equivalently, $\ell_1 + \ell_2 = \ell_3 + \ell_4$.

D. Modifying the Hamiltonian

Performing averages given the extended Kraichnan Hamiltonian of Eq. (8), as it stands, simply recovers the exact expectations for the originating one; any cross-correlations between distinguishable members are identically zero. However, embedding the physical Hamiltonian within a collective description opens a novel degree of freedom for treating interactions. Figure 1 summarizes the whole process. From now on we concentrate on the interaction part of Eq. (8), denoted by $\mathcal{H}_{i;N}$, since the one-body part conveys no new information. We will not consider issues of convergence here; for particular implementations they are carefully discussed in the original papers [14,15].

We can modify the behavior of the interaction part, keeping it Hermitian, by adjoining a factor $\varphi_{\nu_1 \nu_2 | \nu_3 \nu_4}$ such that

$$\mathcal{H}_{i;N}[\varphi] \equiv \frac{1}{2N} \sum_{\ell_1 \ell_2 \ell_3 \ell_4}{}' \langle k_1 k_2 | V | k_3 k_4 \rangle \, \varphi_{\nu_1 \nu_2 | \nu_3 \nu_4} \, a_{\ell_1}^* a_{\ell_2}^* a_{\ell_3} a_{\ell_4}. \tag{9}$$

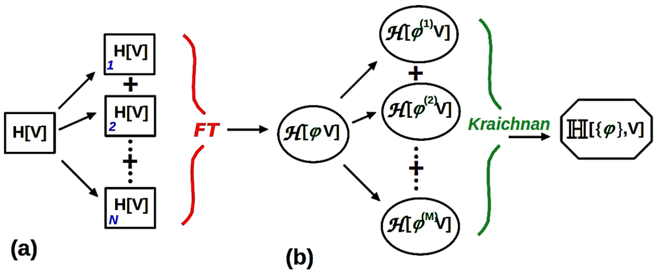

FIG. 1. Construction of the Kraichnan Hamiltonian. (a) The exact many-body Hamiltonian is embedded in a large sum of N identical but distinguishable duplicates. A Fourier transform over the identifying index $n = 1, 2, \ldots, N$ is performed. To each physical interaction potential $\langle k_1 k_2 | V | k_3 k_4 \rangle$ a new parameter $\varphi_{\nu_1 \nu_2 | \nu_3 \nu_4}$ is attached, labeled by the new Fourier indices and transforming in them as does V in its physical indices. (b) The modified Hamiltonian is again embedded in a large sum of M replicas, but each replica is now assigned a unique set of factors φ. The resulting Kraichnan Hamiltonian remains Hermitian. Setting every instance of φ to unity recovers the exact expectations resulting from the original, physical Hamiltonian. If values are specifically structured but otherwise randomly assigned to the M-fold ensemble $\{\varphi\}$, only a selected subset of the physical correlations survives while the rest are suppressed by random phasing.

The expression remains Hermitian if and only if the factor has the same symmetry properties as the potential under exchange of its indices. Thus

$$\varphi_{\nu_4 \nu_3 | \nu_2 \nu_1} = \varphi^*_{\nu_1 \nu_2 | \nu_3 \nu_4}, \quad \varphi_{\nu_2 \nu_1 | \nu_4 \nu_3} = \varphi_{\nu_1 \nu_2 | \nu_3 \nu_4}. \tag{10}$$

The additional procedure of taking expectations will no longer match those for the exact physical Hamiltonian unless, evidently, φ is unity. The crux, however, is that all identities among expectations, dependent on causal analyticity, will still be strictly respected. The Kraichnan Hamiltonian remains well formed in its own right (its Fock space is complete) except that now it describes an abstract system necessarily different from the physical one that motivated it. The task is to tailor it to recover the most relevant aspects of the real physics in reduced but tractable form.

The last step in the logic considers the much larger sum $\mathbb{H}$ of collective Hamiltonians all of the form of Eq. (9), with an interaction part $\mathbb{H}_i$ encompassing a distribution $\{\varphi\}$ of coupling factors prescribed by a common rule:

$$\mathbb{H}_i \equiv \sum_{\{\varphi\}} \mathcal{H}_{i;N}[\varphi]. \tag{11}$$

In Eq. (11) the sum ranges over the prescribed couplings. Each Hamiltonian in the family is Hermitian, so $\mathbb{H}$ must be also. As stated, all physical quantities—with one exception—preserve their canonical interrelationships as their expectations run through φ.

The exception is for identities relying explicitly on the completeness of Fock space associated with $\mathbb{H}$; Kraichnan's ensemble averaging destroys completeness owing to its decohering action. Consider, symbolically, the ensemble projection operator

$$\mathbb{P} \equiv \prod_{\{\varphi\}} \sum_{\Psi[\varphi]} \Psi[\varphi] \Psi^*[\varphi].$$

Overwhelmingly the orthonormal eigenstates of $\mathbb{H}$ will be products of correlated, highly entangled, Kraichnan-coupled superpositions of states in the Fock space of each collective member over the distribution $\{\varphi\}$. Any expectation over the K couplings, directly for $\mathbb{P}$, will cause only those terms to survive whose components in every factor $\varphi_{\nu_1 \nu_2 | \nu_3 \nu_4}$ within $\Psi[\varphi]$ find a counterpart in $\Psi^*[\varphi]$; see Eq. (13) below for the structure of φ. Any other legitimate but off-diagonal cross-correlations interfere mutually and are suppressed. Numerically, the integrity of the Kraichnan projection operator $\mathbb{P}$ is not preserved [20].

Among other things, this loss of coherence leads to a clear quantitative distinction, within the same Φ-derivable approximation, of static (instantaneous) correlation functions over

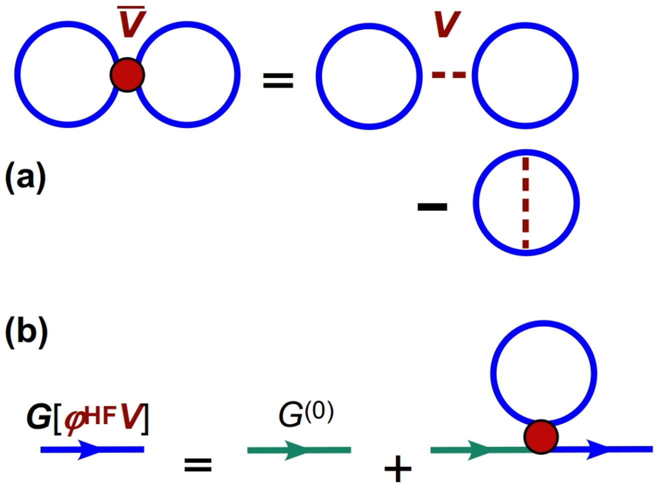

FIG. 2. Scheme for the self-consistent Hartree-Fock interaction energy, derived by insertion into Eq. (12) of the Kraichnan coupling $\varphi^{\rm HF}_{\nu_1\nu_2|\nu_3\nu_4} \equiv \delta_{\nu_1\nu_4}\delta_{\nu_2\nu_3}$. Dots denote the antisymmetrized pair interaction, broken lines the originating potential, and solid lines, one-body propagators. (a) Contributions to the interaction energy. (b) Self-consistency is made evident in the Dyson equation for the single-particle propagator G, where $G^{(0)}$ is the noninteracting counterpart. Nesting of $G:\overline{V}$ in the self-energy contribution means that the bare potential is present to all orders, albeit as a highly reduced subset of the physically exact self-energy.

dynamic ones. Given that distinction, the dynamic and static response functions will still keep their canonical definitions and the sum-rule relations among them are still preserved [16,21].

To align the forthcoming presentation to the notion of crossing symmetry [22] for fermion interactions, we take the further step of antisymmetrizing the potential V. This is readily done in the interaction Hamiltonian, which now reads

$$\mathcal{H}_{i;N}[\varphi] \equiv \frac{1}{2N}\sum_{\ell_1\ell_2\ell_3\ell_4}{}' \varphi_{\nu_1\nu_2|\nu_3\nu_4} \times \langle k_1k_2|\overline{V}|k_3k_4\rangle\, a^*_{\ell_1}a^*_{\ell_2}a_{\ell_3}a_{\ell_4}$$
$$\text{where } \langle k_1k_2|\overline{V}|k_3k_4\rangle \equiv \frac{1}{2}(\langle k_1k_2|V|k_3k_4\rangle - \langle k_2k_1|V|k_3k_4\rangle). \tag{12}$$

Invocations of the pair potential will now refer to Eq. (12). Care has to be taken with signs for composite "direct" and "exchange" objects that turn out actually to be mixtures of both (yet still needing to be topologically distinguished), to make sure the accounting for V itself stays consistent.

We end the review of the Kraichnan formalism by recalling the simplest example for φ generating the exchange-corrected random-phase, or Hartree-Fock, approximation. This choice is $\varphi^{\rm HF}_{\nu_1\nu_2|\nu_3\nu_4} \equiv \delta_{\nu_1\nu_4}\delta_{\nu_2\nu_3}$ [16]. The diagrammatic outcome of this nonstochastic ansatz is illustrated in Fig. 2. The expectation $\langle \mathcal{H}_{i;N}[\varphi^{\rm HF}V]\rangle$ of the interaction energy over $\varphi^{\rm HF}$ consists, almost trivially, of a pair of one-body Hartree-Fock Green functions attached to a single node representing $\overline{V}$.

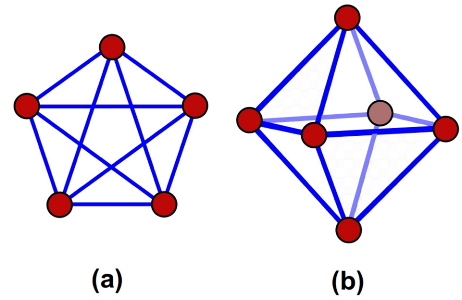

FIG. 3. Two skeleton diagrams for the exact correlation energy not reducible to pairwise-only propagation. (a) Next-order component, beyond first and second in $\overline{V}$, fulfilling the symmetry for Φ derivability but with no two nodes directly linked by a pair of single-particle propagators. (b) Next-higher-order term. Such terms are not generated by any Kraichnan formulation of the pairwise-only parquet Hamiltonian but can be added freely, albeit only *ad hoc*, to its Φ-derivable functional.

The physically richer stochastic definitions of φ, due originally to Kraichnan [14,15], were generalized and adapted in KI [16]. They will again be used in the next section to build up a Kraichnan Hamiltonian for the parquet-generating correlation energy functional and all objects derived from it variationally.

III. A HAMILTONIAN FOR PARQUET

A. The channels and their couplings

In simplest form, the parquet equations take the bare interaction $\overline{V}$ and from it build up all possible iterations that require propagation of pairs of particles from one interaction to the next. This excludes any contributions to the interaction energy functional in which no interaction nodes are directly linked by such a pair; they cannot be broken down into simpler particle-pair processes. Two examples are shown in Fig. 3. We comment later on how these can always be added legitimately but *ad hoc* to the minimal Φ functional of immediate interest.

There are three possible choices of randomized K couplings for φ, each corresponding to the three channels included in parquet: the s channel explicitly selects propagation of pairs of particles, the t channel covers particle-hole pair propagation associated with long-range screening in the random-phase approximation, and its complement, the u channel, describes the Hartree-Fock-like exchange counterpart to t. Recall that while antisymmetrization of the bare potential from V to $\overline{V}$ superposes the actual t and u contributions, one has to continue distinguishing their diagrammatic representations topologically (and their relative sign) to preserve the quantitative outcomes of the Hamiltonian, Eq. (12).

For each possible channel we define a stochastic coupling:

$$\begin{aligned}
&s \text{ channel: } \sigma_{\nu_1\nu_2|\nu_3\nu_4} \equiv \exp[\pi i(\xi_{\nu_1\nu_2} - \xi_{\nu_3\nu_4})], \quad \xi_{\nu\nu'} \in [-1,1] \text{ and } \xi_{\nu'\nu} = \xi_{\nu\nu'},\\
&t \text{ channel: } \tau_{\nu_1\nu_2|\nu_3\nu_4} \equiv \exp[\pi i(\zeta_{\nu_1\nu_4} + \zeta_{\nu_2\nu_3})], \quad \zeta_{\nu\nu'} \in [-1,1] \text{ and } \zeta_{\nu'\nu} = -\zeta_{\nu\nu'},\\
&u \text{ channel: } \upsilon_{\nu_1\nu_2|\nu_3\nu_4} \equiv \exp[\pi i(\vartheta_{\nu_1\nu_3} + \vartheta_{\nu_2\nu_4})], \quad \vartheta_{\nu\nu'} \in [-1,1] \text{ and } \vartheta_{\nu'\nu} = -\vartheta_{\nu\nu'}.
\end{aligned} \tag{13}$$

Their full outworkings are detailed in KI. The uniformly random numbers ξ, ζ, and ϑ are independently distributed; expectations over them mutually decouple and all factors conform to Eq. (10). Each is designed so that, in the stochastic average of the diagrammatic expansion of Φ, product chains whose phases cancel identically from start to finish are immune to the averaging. All other product chains fail to cancel. Being stochastic they interfere destructively, vanishing in the limit of an arbitrarily large ensemble.

With respect to t and u channels, note that an exchange of labels $1 \leftrightarrow 2$ or $3 \leftrightarrow 4$ effectively swaps the definitions and thus the actions of their K couplings. This is consistent with the physics of these channels as mutual exchange counterparts.

In the modality of Eq. (13), σ generates the particle-particle Brueckner-ladder functional while the ring approximation is generated by τ. Last, υ also results in a Brueckner-like functional where particle-hole ladders replace particle-particle ones [16]. There are no other options for pairwise propagation, just as with parquet.

B. Maximal pairwise coupling

None of the K couplings of Eq. (13), alone or in twos, can cover all conceivable scattering arrangements strictly between particle and/or hole propagator pairs. All three must combine sequentially in all possible ways, while preventing any potential replication of terms if two or more K couplings led to the survival of identical Φ terms. To first and second order in $\overline{V}$ one can show that all three elementary couplings generate identical contributions, inducing overcounting which would propagate throughout the nesting of self-energy insertions.

The solution to overcounting is to combine the couplings of Eq. (13) to inhibit any concurrency. We propose the candidate parquet K coupling to be

$$\begin{aligned} \varphi &\equiv 1-(1-\sigma)(1-\tau)(1-\upsilon) \\ \text{so } \varphi_{\nu_1\nu_2|\nu_3\nu_4} &= \sigma_{\nu_1\nu_2|\nu_3\nu_4} + \tau_{\nu_1\nu_2|\nu_3\nu_4} + \upsilon_{\nu_1\nu_2|\nu_3\nu_4} \\ &\quad - (\sigma_{\nu_1\nu_2|\nu_3\nu_4}\tau_{\nu_1\nu_2|\nu_3\nu_4} + \tau_{\nu_1\nu_2|\nu_3\nu_4}\upsilon_{\nu_1\nu_2|\nu_3\nu_4} \\ &\quad + \upsilon_{\nu_1\nu_2|\nu_3\nu_4}\sigma_{\nu_1\nu_2|\nu_3\nu_4}) \\ &\quad + \sigma_{\nu_1\nu_2|\nu_3\nu_4}\tau_{\nu_1\nu_2|\nu_3\nu_4}\upsilon_{\nu_1\nu_2|\nu_3\nu_4}, \end{aligned} \tag{14}$$

preserving overall the Hermitian property specified by Eq. (10).

In any diagram expanded to a given order in $\overline{V}$, the products of K couplings in Eq. (14) may or may not resolve into a set of elementary closed cycles whose multiplicative chain is identically unity when φ averaged (this means, by way of definition, that any subchain hived off within an elementary cycle would necessarily vanish through phase interference). Chains not resolving into a set of independent closed cycles over the contribution will be quenched to vanish in the Kraichnan expectation.

Should two or even three channels have coincident closed cycles, the structure of φ makes certain that the net contribution from this coincidence is always precisely unity; Eq. (14) ensures that there is no overcounting if GG pairings from different channels gave rise to the same diagrammatic structure.

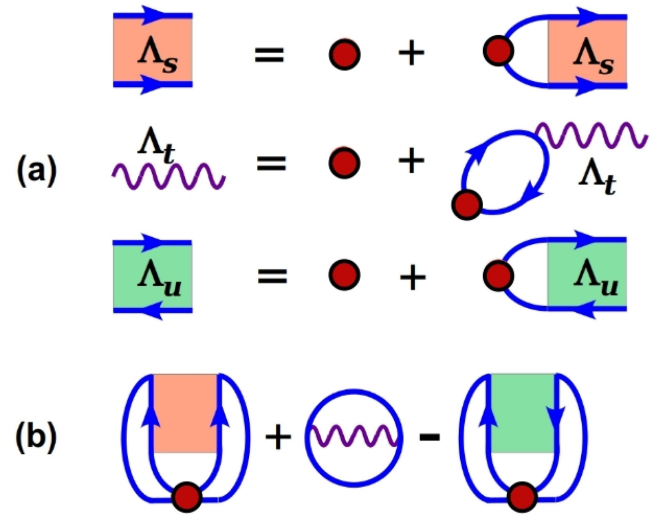

FIG. 4. (a) Definition of the fundamental all-order s, t, and u interactions. Dots denote antisymmetrized pair potential. (b) Symbolic definition of Φ, the correlation energy functional [weightings induced by Eq. (2) are understood], following Kraichnan averaging over all K couplings σ, τ, and υ as in Eq. (14) to remove overcounting when different K couplings lead to identical diagrams. Although the skeleton graphs for Φ appear simple, their complexity is hidden within the self-consistent nesting of self-energy insertions in the propagators (solid lines) according to Eqs. (2)–(4). Since the stu correlation energy is identical to that of the fluctuation-exchange model [6,23], the Kraichnan construction already subsumes the essence of parquet. The combinatorial stu structure is fully revealed only when the response to an external perturbation is extracted (see following).

Such terms can turn up only once in their locations within the expansion for Φ, including iteratively in the self-energy parts.

All allowed pairwise-only combinations of scatterings, and only those, survive the expectation over $\{\varphi\}$ to lead to a legitimate Φ-derivable correlation term with all its symmetries and conserving properties [2,14,16]. The individual energy functional of each component Hamiltonian in Eq. (11), being exact in its particular configuration prior to averaging, automatically has these symmetries in the renormalized expansion of Eq. (2). These are inherited by the diagrammatic structure of every term that survives the taking of expectations and ultimately by the complete averaged Φ.

In Fig. 4(a) we show schematically the structures of the three possible pairwise multiple-scattering combinations contributing explicitly to the correlation energy functional Φ, Fig. 4(b). The K coupling σ leads to the particle-particle Brueckner t matrix Λ_s, while τ leads to the screened interaction Λ_t and lastly υ is the t-exchange complement leading to the particle-hole Brueckner-type ladder Λ_u; this carries an implicit sign change relative to Λ_t owing to the difference of one fermion loop count. From Eq. (14) all processes combine so the renormalized one-body propagators G carry self-energy insertions to all orders in which s, t, and u processes act synergetically, not competing in parallel but entering sequentially.

C. Φ-derivable response

Having arrived at the maximally paired structure of Φ in Fig. 4(b) given the K couplings of Eq. (14), the work of

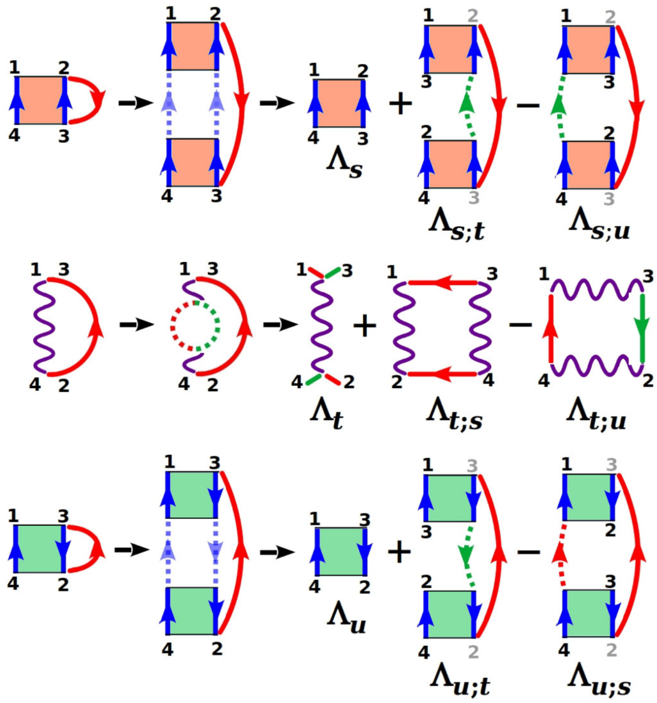

FIG. 5. Systematic removal of a propagator G internal to the self-energy $\Sigma[\varphi\overline{V};G] = \Lambda : G$, after Baym and Kadanoff [1,2], generates the primitive scattering kernel Λ'. Removal of $G(32)$, solid line, simply regenerates Λ. Removing any internal G other than $G(32)$ yields additional terms required for Φ derivability (microscopic conservation). Top line: Beyond the s-channel ladder Λ_s the noncrossing symmetric t-like term $\Lambda_{s;t}$ and u term $\Lambda_{s;u}$ are generated. Middle line: Generation of Λ_t and the nonsymmetric $\Lambda_{t;s}$ and $\Lambda_{t;u}$. Bottom line: Generation of Λ_u with $\Lambda_{u;t}$ and $\Lambda_{u;s}$.

obtaining the parquet equations from it has been done, in one sense, in the analysis detailed by Bickers [6] for the equivalent heuristic FLEX model. However, the Hamiltonian prescription's ramifications lead beyond the derivation of classic parquet.

The goal, then, is to reconstruct a parquetlike scattering amplitude Γ using the ingredients provided by the Kraichnan machinery. We are still left to show its relation to the scattering function Λ, generator of the Φ-derivable diagrammatic stu expansion. While the renormalized structure of Λ seems sparse compared with Γ for parquet [6], the structure for actual comparison is not Λ but begins with the variation

$$\Lambda' \equiv \frac{\delta\Sigma}{\delta G} = \frac{\delta^2\Phi}{\delta G\delta G}, \quad (15)$$

which in fact is the source of the Ward-Pitaevsky identities [19]. One goes from there to set up the complete scattering interaction Γ' for the total system response to a perturbation.

The full outcome of the derivation of Γ' is the dynamical theory of Baym and Kadanoff [2]; in it, conservation entails the additional family of nonparquet diagrams $\Lambda'' = \Lambda' - \Lambda$ shown in Fig. 5. These contribute to every order of iteration. The topologies contained in Λ'' are *not* explicit in the renormalized Λ embedded within $\Phi[\varphi\overline{V};G]$. Not being crossing symmetric they are not permitted, much less generated, within parquet. As with the normal parquet structures that we aim to exhibit from the stochastic Hamiltonian construction, the apparently extra correlation effects, actually mandated by conservation, remain virtual in the renormalized summation for Φ until elicited by an external probe.

Figure 5 details how functional differentiation gives rise to the nonparquet terms, typical of all Φ-derivable descriptions. We want to trace how the purely parquet crossing-symmetric Γ diagrams make up a nontrivial component of the complete set for Γ', the total Baym-Kadanoff response kernel. Γ is not equivalent to Γ'; it is a proper subset [6].

We emphasize the necessary presence, for Φ derivability, of the nonsymmetric components Λ''. These are the approximate system's attempt to match its u terms, for example, with partner terms topologically like the two complementary channels t and s; the same applies correspondingly to the primary s and t terms. However, the question is less why they break antisymmetry but how their presence fits into the cancellation of terms for conservation to govern the model's response.

IV. DERIVATION OF THE PARQUET EQUATIONS

A. Origin within response analysis

To unpack the nested correlations hidden in the renormalized form of Φ we turn to the full Kraichnan Hamiltonian prior to averaging and derive the response to a one-body nonlocal perturbation $\langle k'|U|k\rangle$, which generally will have a time dependence also [1,2]. External perturbations do not couple to the collective index ν but physically only to labels k. The interaction Hamiltonian in Eq. (12) is augmented:

$$\mathcal{H}_{i;N}[\varphi;U] \equiv \sum_{ll'} \langle k'|U|k\rangle a^*_{l'}a_l + \mathcal{H}_{i;N}[\varphi;U=0]. \quad (16)$$

Response to a local field is generated by setting $\langle k'|U|k\rangle \to U(q)\delta_{k',k+q}$, dynamically linking (contracting) the propagators that terminate and start at U.

Physical expectations are taken next, while retaining the individual K couplings φ to keep track of all pair processes. We use matrix notation with repeated indices to expand the intermediate sums.

The two-body Green function is $\delta G/\delta U$ [1]. Working from Eq. (3), vary G^{-1} for

$$\delta G^{-1}(12) = -\delta U(12) - \delta\Sigma[\varphi, G](12)$$

$$\text{or } G^{-1}(12')\delta G(2'1')G^{-1}(1'2) = \delta U(12) + \frac{\delta\Sigma(12)}{\delta G(43)}\frac{\delta G(43)}{\delta U(56)}$$

$$\text{so } \frac{\delta G(21)}{\delta U(56)} \equiv G(25)G(61) + G(21')G(2'1)\Lambda'(1'3|2'4)\varphi_{1'3|2'4}\frac{\delta G(43)}{\delta U(56)},$$

where φ explicitly partners the effective interaction Λ'. There is no overcounting of the s, t, and u contributions of Λ' since, once a line in any self-energy insertion is opened, it will not reconnect to its originating structure but will join instead a new and different (ultimately closed) loop. Symbolically, with I the two-point identity,

$$[II - GG : \Lambda'\varphi] : \frac{\delta G}{\delta U} = GG$$
$$\text{so } \frac{\delta G}{\delta U} = [II - GG : \Lambda'\varphi]^{-1} : GG$$
$$= GG + GG : [II - GG : \Lambda'\varphi]^{-1}\Lambda'\varphi : GG. \tag{17}$$

Recalling Eq. (2), the form of the generating kernel Λ (without the non-crossing-symmetric components from Fig. 5) can be read off from the structure of Φ as in Fig. 4, with the subsidiary kernels Λ_s, Λ_t, and Λ_u:

$$\Lambda = \Lambda_s + \Lambda_t - \Lambda_u$$
$$\text{where } \Lambda_s = \overline{V} + \phi^{-1}\overline{V}\sigma : GG : \Lambda_s\varphi,$$
$$\Lambda_t = \overline{V} + \phi^{-1}\overline{V}\tau : GG : \Lambda_t\varphi,$$
$$\Lambda_u = \overline{V} + \phi^{-1}\overline{V}\upsilon : GG : \Lambda_u\varphi. \tag{18}$$

To put the interactions on the same representational footing as $\overline{V}$, we factor out the outermost K coupling, ϕ. Intermediate chains that cancel right across will finally cancel with ϕ^{-1} appropriate to each channel. In Eqs. (18) the u-channel term of Λ, being the exchange of the t channel, carries the sign tracking the structural antisymmetry of Λ_t on swapping particle (or hole) end points and restoring to V its proper weight of unity in the intermediate summations.

From Eq. (17) the complete four-point amplitude is defined:

$$\Gamma' \equiv \phi^{-1}\Lambda'\varphi : [II - GG : \Lambda'\varphi]^{-1}$$
$$= \phi^{-1}[II - \Lambda'\varphi : GG]^{-1} : \Lambda'\varphi. \tag{19}$$

In terms of Γ' the conserving two-body Green function becomes

$$\frac{\delta G}{\delta U} = GG : [II + \Gamma'\varphi : GG]. \tag{20}$$

B. Parquet equations

At this stage we specialize to the crossing-symmetric subclass of the expansion dictated by Eq. (19). After dropping Λ'' all the crossing-symmetric terms are gathered. The equation is truncated and defines the now crossing-symmetric kernel

$$\Gamma \equiv \phi^{-1}\Lambda\varphi : [II - GG : \Lambda\varphi]^{-1}$$
$$= \phi^{-1}[II - \Lambda\varphi : GG]^{-1} : \Lambda\varphi, \tag{21}$$

keeping in mind that the crossing-symmetric Λ consists only of the primary structures embedded in Φ. While Γ inherits antisymmetry, it forfeits conservation at the two-body level that is guaranteed for Γ' [24].

As with Eq. (19) above, Eq. (21) sums Γ differently from parquet, but the underlying architecture of Γ is the same. In the equation, s, t, and u processes combine in all possible ways while inhibited from acting concurrently. The resolution of Γ becomes a bookkeeping exercise: to make a systematic species by species inventory of all its permissible pair-only scattering sequences, irreducible in the parquet sense, within each channel, finally to weave these into all possible reducible contributions.

In Kraichnan's description one resums Γ by tracking how selective filtering works through the three possible K couplings, while in the parquet approach one enforces, on the intermediate GG pairs, the three distinct modes of momentum, energy, and spin transfer characterizing the s, t, and u channels. Our operation is the same as the pairwise topological argument for Γ in FLEX, detailed in Ref. [6]. To achieve it, the first set of equations isolates the components that are not further reducible within each particular channel:

$$\Gamma_s \equiv \overline{V} + \phi^{-1}\Gamma\tau : GG : \Gamma_t\varphi - \phi^{-1}\Gamma\upsilon : GG : \Gamma_u\varphi,$$
$$\Gamma_t \equiv \overline{V} - \phi^{-1}\Gamma\upsilon : GG : \Gamma_u\varphi + \phi^{-1}\Gamma\sigma : GG : \Gamma_s\varphi,$$
$$\Gamma_u \equiv \overline{V} + \phi^{-1}\Gamma\sigma : GG : \Gamma_s\varphi + \phi^{-1}\Gamma\tau : GG : \Gamma_t\varphi. \tag{22}$$

Manifestly, the components of Γ_s couple only via t or u, excluding any s-channel processes where cutting a pair sequence σGG yields two detached diagrams. Thus, taking the Kraichnan expectation of $(\Gamma_s - \overline{V})\sigma$, nothing survives—and so on for the other channels. The arrangement generates every legitimate convolution involving internally closed cycles of propagation through every channel within Γ while ensuring irreducibility of the three component kernels.

Finally the complete Γ is assembled:

$$\Gamma = \overline{V} + \phi^{-1}\Gamma\sigma : GG : \Gamma_s\varphi + \phi^{-1}\Gamma\tau : GG : \Gamma_t\varphi$$
$$- \phi^{-1}\Gamma\upsilon : GG : \Gamma_u\varphi. \tag{23}$$

In the Kraichnan average only the pairwise terms we have highlighted make it through. Equations (22) and (23) then become identical to the FLEX parquet equations [6]. For each channel the total amplitude can also be recast to reveal its reducibility:

$$\Gamma = \Gamma_s + \phi^{-1}\Gamma\sigma : GG : \Gamma_s\varphi$$
$$= \Gamma_t + \phi^{-1}\Gamma\tau : GG : \Gamma_t\varphi$$
$$= \Gamma_u - \phi^{-1}\Gamma\upsilon : GG : \Gamma_u\varphi.$$

C. Extension of the parquet equations

1. Complete specification of Γ'

The stu-based formalism leads to an interaction energy functional Φ equivalent to the fluctuation-exchange approximation introduced by Bickers *et al.* [23]. The radical difference is that its properties are not imparted intuitively; they are established from a Hamiltonian. The consequence of this canonical provenance is to set a limit on what is possible diagrammatically for a conserving, optimally pairwise-correlated model.

The FLEX model generates the parquet topology naturally by generating, as we have done within Kraichnan's formalism, the variational structure of the Φ-derivable self-energy Σ. Without the additional step of obtaining the perturbative response, the intimate link between the renormalized topology of Φ and the architecture of parquet, which is otherwise implicit within the self-consistent correlation energy functional, does not emerge.

A widespread line of thought in parquet literature assumes there is no distinction between, on the one hand, the scattering kernel Λ in the self-energy Σ and, on the other, Γ acting as the kernel for the total two-body response within parquet. For Φ-derivable models this is not permissible, if only because they yield two different numerical estimates for the static pair correlation function, of which only one meets the exact formulation by functional differentiation of Φ with respect to V [16,21]. This reflects the loss of Fock-space completeness. Later we revisit the implications, for consistency in conservation, of the parquet model's assumption $\Lambda \equiv \Gamma$.

We have a basis to build up more elaborate extensions of the FLEX parquet model following the Kraichnan-based analysis. The complete Φ-derivable, conserving pair-scattering kernel Γ' can now be obtained simply by adapting the parquet equations (22) and (23). Noting that the nonparquet term Λ'' is absolutely irreducible within both parquet and Kadanoff-Baym (recall Fig. 5); the bare potential is replaced with

$$\mathcal{V} \equiv \overline{V} + \Lambda''.$$

Return to Eq. (22), this time to define

$$\begin{aligned}\Gamma'_s &\equiv \mathcal{V} + \phi^{-1}\Gamma'\tau : GG : \Gamma'_t\varphi - \phi^{-1}\Gamma'\upsilon : GG : \Gamma'_u\varphi,\\ \Gamma'_t &\equiv \mathcal{V} - \phi^{-1}\Gamma'\upsilon : GG : \Gamma'_u\varphi + \phi^{-1}\Gamma'\sigma : GG : \Gamma'_s\varphi,\\ \Gamma'_u &\equiv \mathcal{V} + \phi^{-1}\Gamma'\sigma : GG : \Gamma'_s\varphi + \phi^{-1}\Gamma'\tau : GG : \Gamma'_t\varphi, \end{aligned} \quad (24)$$

with the ultimate result

$$\begin{aligned}\Gamma' = \mathcal{V} &+ \phi^{-1}\Gamma'\sigma : GG : \Gamma'_s\varphi + \phi^{-1}\Gamma'\tau : GG : \Gamma'_t\varphi\\ &- \phi^{-1}\Gamma'\upsilon : GG : \Gamma'_u\varphi.\end{aligned} \quad (25)$$

We stress that the only feature that matters now in Eqs. (24) and (25) is the topological arrangement of the elements of the response kernel, exhausting all possible interplays among the three Φ-derivable channels independently of crossing symmetry.

Now we address the addition to the energy functional, presumably by physical reasoning, of absolutely pair-irreducible graphs for Φ. (Two are shown in Fig. 3.)

2. Contributions from pair-irreducible correlations

Primitive additions to Λ' can be incorporated once again via Eqs. (24) and (25). In Φ derivability the choice of symmetric structures for the Λ kernel is highly constraining. Readers can convince themselves, with a bit of sketching, that no such three-node term exists. Nor is there an stu-irreducible four-node term for Φ that has the needed symmetry. Whereas the crossing-symmetric four-node "envelope" graph depicted in Fig. 6(a) is a valid irreducible interaction in parquet [6], when incorporated as a fully closed diagram it must carry inequivalent propagators, making it inadmissible in any Φ-derivable subset of the correlation energy.

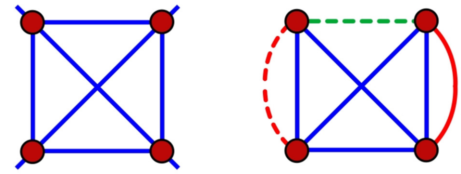

FIG. 6. (a) Fourth-order stu-irreducible crossing-symmetric graph, valid as a primitive input to the standard parquet equations but not Φ derivable. While the graph can be generated by removing an interaction node from its analog in Fig. 3(a), when closed with two final propagators as in (b) it is forced to carry inequivalent propagators (dotted lines). Thus it is disqualified from any Φ-derivable approximation since it cannot lead to a unique self-energy functional.

The next-order Φ-derivable skeleton beyond second is that of Fig. 3(a), with five interaction nodes. Its variation with respect to any node—removal of a node from Fig. 3(a)—generates a two-body correlation with parquet's envelope graph as its kernel. However, there is no systematic link between such a variation and parquet.

The issue with adding higher-order stu-irreducible terms to Φ, again assuming that they held some novel physical effects, is that one gets back to adding many-body correlations heuristically, without a Hamiltonian basis. Strictly, then, the sum-rule identities no longer come for free but require individual validation (this has been done up to the third-frequency-moment rule [21]). Kraichnan's procedure is limited to pair interactions; so far, it is hard to envisage how any Hamiltonian extension could generate these additional complex objects. Nevertheless, adding a totally pairwise-irreducible structure satisfying Baym-Kadanoff symmetry will not spoil Φ derivability.

D. Parquet and Φ derivability

In establishing full parquet the Φ-derivable FLEX approximation has been taken as a suitable entry point for successive iterations aimed at approaching the full structure, but the initial self-energy $\Lambda : G$ is considered to fall short of a maximally correlated parquet. It is deemed necessary to feed the FLEX-derived crossing-symmetric Γ in Eq. (23) back into Σ in Eq. (4) via the replacements [6] (ensuring that $G : \Gamma : G$ does not double up on terms previously included)

$$\Sigma(13) \leftarrow \widehat{\Gamma}(12|34)G(42)$$

in which
$$\begin{aligned}\widehat{\Gamma}(12|34) \leftarrow\; &\overline{V}(12|34)\\ &+ \Gamma(12|3'4')G(4'2')G(3'1')\overline{V}(1'2'|34),\end{aligned} \quad (26)$$

with the nonconforming piece, $\Gamma'' = \Gamma' - \Gamma$, naturally absent. Substitution of $\widehat{\Gamma}$ for Λ in the self-energy assumes that no distinction should be made between the approximate self-energy kernel and the approximate two-body response kernel: that, as in the exact theory, they are one and the same [5,6]. As a generator of new primitively irreducible structures Eq. (26) can be iterated at will.

In view of how the generic parquet equations (24) and (25) always build up from at least the leading primitive irreducible, namely, $\overline{V}$, any resulting Γ must always incorporate Λ from Eq. (18). Reopening lines in the self-energy $\widehat{\Gamma}[V, G] : G$ is always going to regenerate pieces including the unwanted nonparquet term Λ''.

To compare the behaviors of the different self-energy kernels for stu and standard parquet, we use a result of Luttinger and Ward [17]. Equation (47) of that reference provides an alternative formulation of the correlation energy when Λ in Eq. (2) is the exact Γ interaction:

$$\Phi[V;G] = -\langle \ln(I - G^{(0)} \cdot \Sigma \cdot) \rangle - G[V] : \Sigma + \int_0^1 \frac{dz}{2z} G[V] : \Gamma[zV; G[V]] : G[V]. \quad (27)$$

The difference between the coupling-constant integral on the right-hand side of this identity and its counterpart in Eq. (2) is that the former keeps track only of the combinatorial factors for the Vs in the original linked skeleton diagrams $\Gamma[V; G^{(0)}]$ but now with $G[V]$, containing V at full strength, in place of each bare line $G^{(0)}$. By contrast, in the integral on the right-hand side of Eq. (2) the coupling factor attaches to all occurrences of V, that is, including those within $G[V]$ itself.

The correlation energy as given in Eq. (27) leads to two identities. Exploiting the equivalence of all propagators in the closed structure G: Γ: G within the integral, varying on both sides with respect to the self-energy gives

$$\begin{aligned} \frac{\delta\Phi}{\delta\Sigma} &= (I - G^{(0)} \cdot \Sigma)^{-1} \cdot G^{(0)} - G \\ &\quad - \frac{\delta G}{\delta\Sigma} : \Sigma + \frac{\delta G}{\delta\Sigma} : \Gamma[V; G] : G \\ &= -\frac{\delta G}{\delta\Sigma} : (\Sigma - \Gamma[V; G] : G) \\ &= 0 \end{aligned} \quad (28)$$

on using Eq. (4). In vanishing identically, the derivative establishes the correlation energy as an extremum with respect to perturbations, as these add linearly to Σ.

Next,

$$\begin{aligned} \frac{\delta\Phi}{\delta G} &= ((I - G^{(0)} \cdot \Sigma)^{-1} \cdot G^{(0)} - G) \cdot \frac{\delta\Sigma}{\delta G} + \Gamma[V; G] : G \\ &= \Sigma. \end{aligned} \quad (29)$$

Consistency with Eq. (4) is confirmed.

We look at how Eq. (27) works in the Φ-derivable case. Since it applies canonically in the case of the full Kraichnan Hamiltonian, the form survives the expectation over the stu couplings, as will the form of the variational derivatives; the skeletal topology of the integrals on the right-hand sides of Eqs. (2) and (27) is the same. In the stochastic expectations on the right-hand side of Eq. (27), Γ goes over to the reduced stu structure Λ depicted in Fig. 4. This is because, in the coupling-constant integral, the pattern of surviving and suppressed products of factors φ is identical with that leading to Eq. (2).

Define the Φ-derivable correlation energy $\Phi_{\rm KB}$ from the corresponding Eq. (27). All propagators in the structure G: Λ: G are equivalent. The variation in Eq. (28) again leads to

$$\frac{\delta\Phi_{\rm KB}}{\delta\Sigma} = -\frac{\delta G}{\delta\Sigma} : (\Sigma - \Lambda : G) = 0 \quad (30)$$

so the extremum property holds for the approximate correlation energy. Equation (29) becomes

$$\frac{\delta\Phi_{\rm KB}}{\delta G} = \Lambda : G = \Sigma \quad (31)$$

since the symmetry of the integral $G : \delta\Lambda/\delta G : G$ works once more as for Eq. (4) to recover the self-energy.

The analysis is now applied to the classic parquet expansion, whose candidate correlation energy functional, defined from Eq. (27), we will call $\Phi_{\rm PQ}$. In this instance one gets

$$\begin{aligned} \frac{\delta\Phi_{\rm PQ}}{\delta\Sigma} &= -\frac{\delta G}{\delta\Sigma} : (\Sigma - \Gamma[V; G] : G - \Delta\Gamma[V; G] : G), \\ \Delta\Gamma[V; G] &\equiv \int_0^1 \frac{dz}{z} (\Gamma[zV; G[V]] - z\Gamma[V; G[V]]) \\ &\quad + \int_0^1 \frac{dz}{2z} \frac{\delta\Gamma[zV; G[V]]}{\delta G} : G[V]. \end{aligned} \quad (32)$$

This does not vanish because the parquet structure $G : \Gamma : G$ contains inequivalent propagators. Therefore Eq. (28) fails. The same topological absence of Φ-derivable symmetry spoils the complementary attempt to define $\Phi_{\rm PQ}$ from the alternative fundamental expression of Eq. (2).

Figure 7 typifies the issue. At third order in the bare potential the parquet iteration of Γ obtained from FLEX produces a new absolutely irreducible term at fourth order whose skeleton

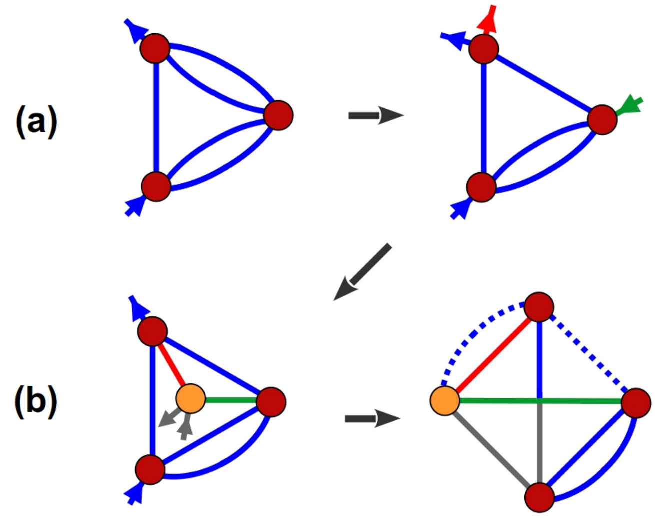

FIG. 7. The iterative parquet algorithm, Eq. (26), starting from the FLEX self-energy, is incompatible with Φ derivability. (a) Differentiation of the self-energy term at third order in the interaction gives a term in the parquet kernel series. (b) Iteration of the self-energy in the parquet algorithm must close the structure from (a) by adding an interaction, avoiding overcounting of reducible terms. This generates a novel irreducible component in the parquet series. A final closure generates the linked correlation-energy diagram of Fig. 6(b), which is not a legitimate Φ-derivable contribution. Since Φ derivability must hold at every order, no level of iteration of the parquet kernel can fulfill it.

contribution to Φ would carry inequivalent propagators, as already shown in Fig. 6(b). Since the symmetry leading to a well-defined Φ must be present at all orders it follows that no formulation of parquet, built on pairwise-only scattering, can be Φ derivable. Conversely, the stu construction *à la* Kraichnan is the only strictly pairwise-correlated model that has a Hamiltonian basis while exhibiting the essential parquet topology.

The failure of Eq. (32) to vanish has the more serious implication that a parquet model does not correspond to a system with a well-defined ground-state energy. Securing that would require a Φ_{PQ} conforming to the criteria of Baym and Kadanoff. If such a functional can be constructed to satisfy Eq. (29), say, it will not have the canonical Luttinger-Ward form of either Eq. (2) or Eq. (27). The question of the existence of a stable ground-state configuration stays undecided for parquet.

So far we have shown how both Φ-derivable and parquet models fail to produce forms for the correlation energy that are fully consistent both with respect to conservation and to crossing symmetry. However, unlike parquet, Φ derivability preserves internal consistency in the sense of Luttinger and Ward [17], in particular Φ as an extremum with respect to external perturbations.

Our conclusions on the limits of both parquet and Φ-derivable models coincide fully with those of the diagrammatic analysis of Smith [11]. That analysis applies as well to more elaborate Φ-derivable structures beyond the one corresponding to stu or FLEX, underwritten by its Kraichnan Hamiltonian. In his different functional-integral approach, oriented towards critical behavior, Janiš [12,13] likewise remarks on the discrepancy between the parquet kernel's analytical properties and those obtained from Φ derivability.

E. Crossing symmetry and response

Notionally, while crossing symmetry will apply to scattering off an open system, response analysis concerns a closed system and thus a different interplay of two-body vertex and one-body self-energy correlations. Any complement to the extra term Γ'', if found neither in Γ itself nor in the self-energy insertions subsumed in the total two-body response, could make no contribution to that conserving response within its approximating Φ-derivable framework. If needed for conservation, the counterterm must show up somewhere [25].

Specializing to the purely computational aspect of the stu and parquet analyses, we draw attention to Fig. 2 of the paper by Glick and Long [25], here replicated in Fig. 8. It exhibits the dominant high-frequency contributions to the imaginary (damping) part of the polarization function for the electron gas and derives from the bare expansion of the density response, generated by $\delta^2\Phi/\delta U \delta U$ when the exact correlation energy is truncated at second order in the bare potential V. Self-energy insertions from the externally coupled propagators must be computed in systematic superposition with the corresponding interaction-vertex contributions.

Glick and Long's example demonstrates that, to account systematically for the dynamical correlations in the response, self-energy contributions from the propagators external to the two-body interaction Γ enter, as well as those internal to it. This means that a protocol broader than explicit crossing symmetry determines the bookkeeping that produces the overall conserving result. In the Φ-derivable approach, a similar pattern of cancellation also provides the counterbalancing mechanism for the nonparquet component Γ''.

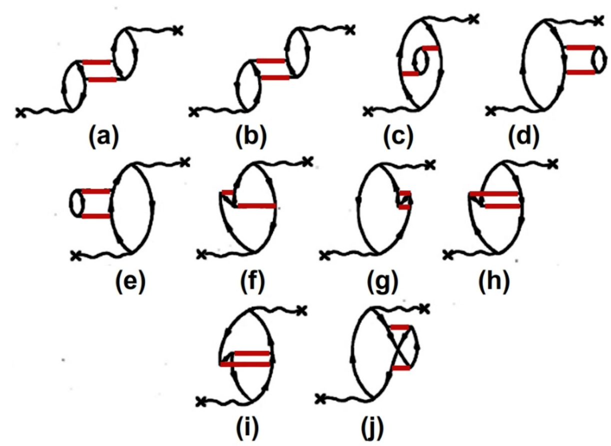

FIG. 8. Damping terms in the conserving high-frequency summation of the two-body electron-gas polarization function, exact to second order in V (solid horizontal lines), after Fig. 2 of Glick and Long [25]. Wavy lines terminating with **x** are couplings to the external probe; directed lines are free propagators. Terms (a), (b), (c), (f), (h), and (i) have their kernel in Λ' as generated from Φ. For consistency, these two-body vertex components are summed concurrently with the one-body insertions (d), (e), (g), and (j) that come from the uncorrelated bubble GG. The overall topology in terms of bare lines does not discriminate between self-energy and vertex terms, and its systematic cancellations rely on more than manifest crossing symmetry.

The following is of interest. The Φ-derivable model, truncated beyond second order in $\overline{V}$, reproduces precisely the diagrams of Fig. 8. At second order, the structure of the kernel Λ of Φ is ambiguously defined (degenerate, if one likes); it may be envisaged to manifest in any of the channels s, t, or u, which is the very reason for forming the composite K coupling of Eq. (14) to avoid overcounting. Nevertheless, perturbing the system lifts the structural degeneracy, with all three channels emerging on an equal footing in the Kadanoff-Baym functional derivation of the second-order kernel Λ'. In this quite special case Γ' is crossing symmetric, yet crossing symmetry is not uniquely assignable to the generating kernel Λ. Beyond second order the channel ambiguity is lifted and crossing symmetry for Λ' is lost; but what the second-order case highlights is that the stu parquet structure is inherent in Φ derivability, even if in a weaker sense and even if insufficient to secure strict crossing symmetry in general. One can refer to Fig. 5 to see this stated graphically.

Equation (2) for the correlation energy implies that its fundamental expansion is in powers of the underlying bare interaction V regardless of where it occurs structurally. This implies in turn that one should look again at the expansion in terms of the bare propagator $G^{(0)}$ rather than focus exclusively of the full propagator G. As indispensable as G is as a construct in making sense of the correlation physics, it tends to hide those instances of V within the propagators that counterbalance its presence in the skeleton graphs defining the vertex components; a concealment that, as suggested by Fig. 8, masks how cancellations pair up among two-body and one-body self-energy elements.

The parquet model's self-energy structures for G are set by crossing symmetry through the feedback imposed on the self-energy kernel. There, it is the skeletal topology of Γ that governs the processes of cancellation. For Γ' in the complete Φ-derived two-body Green function, conservation operates otherwise: as in Fig. 8, competing effects must cancel in a determinate superposition. It is this that conditions the topology of the approximate Γ', not the other way around.

Since G is an infinitely nested functional of V, the renormalized Λ and Γ' can well differ diagrammatically while their bare-expansion analogs, respectively $\widetilde{\Lambda}$ and $\widetilde{\Gamma}'$, will not. These last two cannot differ in their structure because the *only* topological distinction between the bare graphs of Φ and the bare graphs of the derived correlated response is the external perturbation nodes attached to (at least) a pair of bare propagators. In other words,

$$\widetilde{\Gamma}' = \widetilde{\Lambda}.$$

By themselves, the internal arrangements of the renormalized four-point kernel are insufficient for response. One needs the entire physical object $\delta G/\delta U$ and not simply $\delta^2\Phi/\delta G\delta G$. The response function's graphs are closed: it is a contraction of the two-body Green function [1]. The outer connections of Γ' must terminate in two particle-hole pairs GG to obtain the dynamically correlated contribution. In the overall accounting the leading uncorrelated particle-hole bubble GG also plays an explicit role.

The physical response function is the same whether written in terms of $\widetilde{\Gamma}'$ or of Γ'. It follows that in the latter's renormalized setting the nonparquet component Γ'', embedded in the complete response, finds its canceling counterparts among the self-energies. For standard parquet, despite the bootstrap equation (26), the self-energy terms in the internal propagating pairs GG are not necessarily tuned to overall cancellation; crossing symmetry reflects only the skeletal form of Γ, not its dynamics. It is an additional assumption that cancellations in parquet are looked after automatically. In practice, they are not. Figure 8 gives a clue as to why.

V. SUMMARY

We have recovered the parquet equations from an augmented form of Hamiltonian within Kraichnan's fundamental stochastic embedding prescription [14,15]. Our particular reinterpretation of the parquet model inherits the entire suite of conserving analytic (causal) identities from the exact many-body description for its generating model Hamiltonian. Relations that rely explicitly on Fock-space completeness are not preserved, since Kraichnan averaging must decohere classes of interaction-entangled multiparticle states (for example, structures as in Fig. 3).

On the way we have examined the seeming paradox of a fully conserving pairwise-maximal Φ-derivable theory with crossing-symmetric kernel yet leading to a nonsymmetric response kernel on one side (while still including standard parquet in its structure), and on the other the pairwise-maximal parquet theory in both elementary and iterated forms, maintaining crossing symmetry but not conservation. This prompts thought on which philosophy to follow in formulating many-body approximations, and for which purpose.

The second lesson of this work goes to a conception of how model correlation theories operate vis-à-vis the conservation laws in a system closed to external particle exchange. In understanding fluctuations and response, the parquet construction can be applied fruitfully within a canonically founded perspective that respects parquet's pairwise-maximal topology in logical independence from manifest crossing symmetry, inherited from the distinct open-system physics of nuclear scattering.

In nuclear scattering, at any rate conceptually [22], free fermionic constituents arrive from asymptotic infinity to encounter an open assembly of the same species. They interact strongly and the free final products scatter off to infinity. One then expects the outcome to be governed by the optical theorem, crossing symmetry, and thus the forward-scattering sum rule [8].

In a setting such as transport, the boundary conditions are different; the problem involves constituents that are always confined to the medium, interacting collectively and strongly while coupling weakly to an external perturbing probe. A closed scenario interrogates the system very differently. Accounting of the self-energy contributions from the initial and final particle-hole GG pairs as well as the uncorrelated bubble GG, coupled via the probe, now matters, and reflects the main philosophical difference between standard parquet and its Φ-derivable rereading in the ambit of response. The role of the vertex terms demands attention to systematic counterbalancing from the self-energy terms, including from incoming and outgoing particle-hole states. Such processes are ensured in Φ derivability, while in parquet they are assumed.

The elegant application of crossing symmetry to particle-antiparticle processes, fusing them seamlessly with the less problematic but structurally disparate particle-particle pair processes, is a foremost idea in many-body understanding. For Φ derivability defined by a Hamiltonian, centered upon conservation and oriented towards response, one is led to a violation of crossing symmetry in the derived stu scattering kernel. In the context of self-energy-versus-vertex accounting, this may be offset partly through the pattern of mutual cancellations ensuring conservation.

A fully conserving parquet response theory, no longer crossing symmetric but sharing the identical pairwise-only arrangement of the original parquet equations, emerges naturally from the Hamiltonian description of the stu or FLEX approximation. The caveat is that, in it, the correlation-energy kernel Λ and the scattering kernel Γ' functionally derived from it remain distinct in playing distinct roles in the renormalized physics. If their differing structures are conflated, conservation fails.

The puzzle remains. Φ derivability in an approximate expansion leads to crossing-symmetry violations, yet in maintaining conservation it suggests that the violating components are systematically canceled by other means. Imposing crossing symmetry on an approximating subset of the two-body scattering amplitude would seem to take care of systematic cancellation, yet not in a way that conserves [26]. Understanding in greater detail just how cancellation acts would therefore provide a much needed clarification.

How might Kraichnan's idea in itself be taken further? First, the present analysis is readily extended both to nonuniform cases and at least to some instances where singular behavior in any of the pair channels may break ground-state symmetry. Applying it to analyze nonperturbative many-body formalisms is also promising. Variational and coupled-cluster methods are potential candidates. The stochastic embedding approach pioneered by Kraichnan may not be the only way to set approximate many-body approaches on a canonical footing. However, the power of the method in guaranteeing all the conserving analytic identities that link one- and two-body correlation functions, even in approximation and beyond linear response, speak compellingly for revisiting an original and penetrating analysis long celebrated in the turbulence-theory community [27] yet, with rare exceptions, [2] largely unnoticed by its sister community of many-body theory.

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[20] One can look at the coherence loss differently. Analyticity via the Kramers-Krönig relations generates a set of odd-frequency moment identities involving the dynamic structure factor. This includes the first-moment longitudinal f sum and conductivity sum rules [18]: generic identities that survive the Kraichnan expectation operation because their analytic structure survives it. However, the even-frequency moments are model dependent in a way that the odd-moment identities are not. Unlike the latter, the even-moment integrals decouple from the constraint of causality. In the exact case the leading such expression ties the static structure factor, an equilibrium object, to the zero-moment frequency integral of the dynamic structure factor, that is, the nonequilibrium response. The static structure factor is determined by the functional derivative of Φ with respect to V and can be resolved with the projection operator, whose entangled character is partially destroyed in the Kraichnan expectation. The nonequilibrium object expresses actually a richer level of entanglement (compare Figs. 4 and 5 in the text) and does not resolve in the same way, so its frequency integral gives a different result. In a Φ-derivable model the zero-moment relation between static and dynamic structure factors is no longer valid; in sharp contrast the third-moment sum rule, relating them through analyticity, still holds [21].
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[26] The dilemma invites restatement of our previous point: in theories of condensed systems one invokes periodic boundary conditions (that is, a running-wave basis) over an arbitrarily large yet still spatially bounded assembly. Implicitly, this imposes a confining potential on the basis states defining the Hamiltonian in analogy with the infinite square well. Real open systems, such as molecules and nuclei, are more akin to the finite square well; there are not only bound states but asymptotically free ones as well. In the first context, Φ derivability does not make room for the existence of free states in that sense; the implicit confinement is global and admits only a many-body ground state that can be perturbed but not disrupted. In the second context, existence of genuinely unconfined states leads to a many-body scattering scenario that does *not* correspond to the relatively low-lying excitations out of the ground state, but is radically altered. It can be argued then that parquet, though in no way deficient as a dynamical model in itself, would be misapplied to a confined system's ground state and its excitations (with standard boundary conditions). Correspondingly Φ derivability, a description of the ground state with

fluctuations, would be misapplied if the physical setting involved asymptotically free dissociated states that did not exist in its underlying Fock space. A Hamiltonian model leading to formal Φ derivability can certainly be constructed for an open system with asymptotically free states, but its computation would be much more challenging.

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Correction: The previously published Figure 5 contained an error in the direction of two arrows and has been replaced. A sign error in Eq. (32) has been fixed.