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Proceedings of the International Summer School on

Nucleon-Nucleon Interaction and Nuclear Many-Body Problems

Changchun, China
July 1983

Editors: S. S. Wu
T. T. S Kuo

Associate Editors: Y. Z. Zhuo
Z. Y. Zhang
S. D. Yang

World Scientific

Published by

World Scientific Publishing Co Pte Ltd.
P O Box 128
Farrer Road
Singapore 9128

ISBN 9971-966-35-2
9971-966-46-8 pbk

Printed in Singapore by Koon Wah Printing Pte. Ltd.

LINEAR RESPONSE AND SUM RULES IN THE COUPLED-CLUSTER FORMALISM*

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Lecture presented at the
International Summer School on Nucleon-Nucleon Interaction
and the Nuclear Many-Body Problem
held at Changchun, China
July 25 — 31, 1983

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* Supported in part by the U.K. Science and Engineering Research Council.

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1. INTRODUCTION

In earlier lectures at this Summer School, Professor Kümmel has spoken in some detail about the fundamental development and applications of the exp(S) or coupled-cluster formalism (CCF) of quantum many-body theory. It should be clear from these lectures that the CCF is strongly anchored to the hamiltonian of the system under consideration, and indeed this has been one of its underlying sources of strength. It is however not surprising therefore that calculations of quantities other than ground-state (g.s.) and excited-state (e.s.) energies, and other quantities easily accessible through the Schrödinger equation, have been slower to be developed. Indeed, most of what Professor Kümmel has spoken about here can be characterised as a cluster decomposition (for both the g.s. and e.s. cases separately) of the many-body Schrödinger equation.

What I intend to discuss in this lecture is a recent development at Manchester of the CCF[1]) in which we have succeeded in imbedding the well-known theory of linear response within this formalism, and have shown how out of it emerges a whole new hierarchy of very useful sum rules. One outcome of this work is that it now provides a very valuable bridge between the otherwise somewhat disjoint, although clearly intimately related, g.s. and e.s. formalisms, and also gives a set of independent yardsticks against which approximations in both formalisms can be assessed for mutual compatibility. The new formalism will also allow any extra information that we possess (either from experiment or other theoretical frameworks) about either the excitation spectrum or the g.s. correlations of the many-body system, to be used to extract information within the CCF on the other.

2. THE SCHRODINGER EQUATION AND ITS CCF DECOMPOSITION

While not wishing to repeat too much of what Professor Kümmel has already described in detail, it will be useful for us first to consider from our new perspective such of the main elements as will be needed later of the CCF applied to both the g.s. and e.s. Schrödinger equation.

For simplicity and ease of exposition, the entire ensuing discussion is given for infinite $(N \to \infty)$ homogeneous systems of bosons. The later extension to Fermi systems is, in principle at least, straightforward!

2.1 The ground-state CCF

A convenient starting-point for the g.s. CCF[2-9] is the usual exp(S) expression for the exact g.s. N-body wavefunction $|\Psi\rangle$,

$$|\Psi\rangle = e^{S}|\Phi\rangle \quad ; \quad S = \sum_{1}^{N} S_n \quad , \tag{1}$$

in terms of an arbitrary N-body model (or reference or uncorrelated) state $|\Phi\rangle$ which we shall choose for simplicity to be a single-state (usually zero-momentum) boson condensate,

$$|\Phi\rangle = (N!)^{-\frac{1}{2}}(b_0^\dagger)^N|\mathrm{vac}\rangle \quad , \tag{2}$$

where $|\mathrm{vac}\rangle$ is the vacuum state and o labels the condensate-state. In terms of a complete set of boson creation operators $b_\alpha^\dagger$, which create the (arbitrary) complete orthonormal single-particle (s.p.) basis $|\alpha\rangle$ when acting on $|\mathrm{vac}\rangle$, the correlation operators S_n, which excite n particles from the condensate into "normally unoccupied" (particle) states, leaving n condensate-hole states, may be written as

$$S_n = (n!)^{-1} \sum_{\rho_1 \cdots \rho_n} b_{\rho_1}^\dagger \cdots b_{\rho_n}^\dagger (N^{-\frac{1}{2}} b_0)^n \, S_n(\rho_1 \cdots \rho_n) . \tag{3}$$

In Eq. (3) and elsewhere, the labels $\rho_1 \cdots \rho_n$ indicate non-condensate (or particle) states, and Eq. (3) thus displays the linked-cluster aspect of the original exp(S) ansatz of Eq. (1).

The g.s. coupled-cluster equations are now formally derived in two simple steps. The g.s. Schrödinger equation with energy eigenvalue E, is first pre-multiplied by the operator exp(-S) as a formal step which eliminates from the outset some "unlinked" terms which otherwise have to be specifically removed later; and secondly the scalar product is then taken either with the model state $|\Phi\rangle$ or with the n particle-hole states,

$$b_{\rho_1}^\dagger \cdots b_{\rho_n}^\dagger (N^{-\frac{1}{2}} b_0)^n |\Phi\rangle \quad . \tag{4}$$

The states $|\Phi\rangle$ and (4) clearly span the entire N-boson Hilbert space

when n runs from 1 to N, and when the labels ρ_i run over all (non-condensate) states of the complete s.p. basis. Thus, the resulting equations,

$$\langle\Phi|e^{-S}He^{S}|\Phi\rangle = E \ , \tag{5a}$$

$$\langle\Phi|(N^{-\frac{1}{2}}b_0^{\dagger})^n b_{\rho_n}\cdots b_{\rho_1}e^{-S}He^{S}|\Phi\rangle = 0 \ , \tag{5b}$$

which are the g.s. coupled-cluster equations are fully equivalent to (and just a cluster decomposition of) the g.s. N-boson Schrödinger equation. Further evaluation of Eqs. (5) is straightforward although algebraically tedious. For example, in a momentum-eigenstate (plane-wave) s.p. basis, and taking the model state to be the zero-momentum condensate, we find that $S_1 \equiv 0$ by momentum conservation, and Eqs. (5a) and (5b) in the case $n = 2$, reduce respectively in the case of a hamiltonian containing local pairwise interaction potentials only, with a momentum-space representation as $V(q)$, to:

$$\frac{E}{N} = \tfrac{1}{2}NV(0) + \tfrac{1}{2}\sum_{\vec{q}} V(q)S_2(q) \ , \tag{6a}$$

$$\frac{\hbar^2q^2}{m}S_2(q) + NV(q)[1+S_2(q)]^2 + (-4\frac{E}{N})S_2(q) + \sum_{\vec{q}'} V(\vec{q}-\vec{q}')S_2(q') + \sum_{\vec{q}'} V(q')[2N^{\frac{1}{2}}S_3(\vec{q},\vec{q}',-\vec{q}-\vec{q}') + \tfrac{1}{2}NS_4(\vec{q},-\vec{q},\vec{q}',-\vec{q}')] = 0 \ , \tag{6b}$$

where $S_2(q) \equiv S_2(\vec{q},-\vec{q})$. The five terms in Eq. (6b) represent respectively (i) the kinetic energy (KE) contribution; (ii) the term that, with the KE, generates the random-phase approximation (RPA); (iii) the term that generates the fully self-consistent energy insertions on the bare zero-momentum condensate propagator (i.e., the boson analogue of the fermion "hole-potential"); (iv) the term that repeatedly scatters two particles outside the condensate and hence generates the two-particle ladder diagrams and the associated Bethe-Goldstone equation; and finally (v) the coupling terms to three - and four-body clusters.

Of course, in order to be useful in practice, one has to truncate the hierarchy of Eqs.(5b), and I remind you only of the "natural" truncation of the so-called SUBn scheme wherein each of the amplitudes S_i is set to zero for $i > n$, and the remaining n coupled, nonlinear equa-

tions are solved for the subsystem amplitudes $S_n(\rho_1 \cdots \rho_n)$ with $i \leq n$.

2.2 The excited-state CCF

As described above the g.s. CCF presumably relates not only to the g.s. but also to those excited states with the same relevant quantum numbers as the g.s. that have non-zero inner product with the model state $|\Phi\rangle$. In this context we note that Eqs. (1) and (3) automatically provide a normalization $\langle\Phi|\Psi\rangle = 1$. To proceed therefore, we may restrict ourselves to excited states $|\Psi_\ell\rangle$ which are orthogonal to both $|\Phi\rangle$ and $|\Psi\rangle$. Emrich[10] has then shown that an appropriate (linked) choice of e.s. CCF wavefunction is

$$\begin{aligned} |\Psi_\ell\rangle &= S^{(\ell)} e^S |\Phi\rangle \quad ; \quad S^{(\ell)} = \sum_1^N S_n^{(\ell)} \quad , \\ S^{(\ell)} &= (n!)^{-1} \sum_{\rho_1 \cdots \rho_n} b^\dagger_{\rho_1} \cdots b^\dagger_{\rho_n} (N^{-\frac{1}{2}} b_o)^n S_n^{(\ell)}(\rho_1 \cdots \rho_n) \quad , \end{aligned} \tag{7}$$

where each nonzero vector $S_n^{(\ell)}|\Phi\rangle$ is assumed to have a nonzero inner product with $|\Psi_\ell\rangle$. If the excited state is a momentum eigenstate with eigenvalue $\vec{q}$, and if we choose again to work in a plane-wave s.p. basis, the implication of this is that the s.p. momenta $(\rho_1 \cdots \rho_n) \rightarrow (\vec{k}_1 \cdots \vec{k}_n)$ in Eq. (7) must sum to $\vec{q}$, whereas in the g.s. Eq. (3) they must sum to zero.

The e.s. CCF equations are now again easy to derive formally. In order to eliminate the g.s. energy level E, the e.s. Schrödinger equation with energy eigenvalue $E_\ell \equiv E + \omega_\ell$ is first combined with the g.s. equation to give

$$[H, S^{(\ell)}]|\Psi\rangle = \omega_\ell S^{(\ell)}|\Psi\rangle \quad , \tag{8}$$

in terms of the excitation energy, ω_ℓ. A similar procedure as in the g.s. case then leads to the linked CCF e.s. equations,

$$\langle\Phi|(N^{-\frac{1}{2}} b_o^\dagger)^n b_{\rho_n} \cdots b_{\rho_1} e^{-S}[H, S^{(\ell)}]e^S|\Phi\rangle = \omega_\ell S_n^{(\ell)}(\rho_1 \cdots \rho_n) \quad , \tag{9}$$

as the counterpart of the g.s. Eqs. (5). The e.s. equations thus take the form of a coupled set of linear eigenvalue equations for the e.s. subsystem amplitudes $S_n^{(\ell)}(\rho_1 \cdots \rho_n)$ with the same excitation energy eigenvalue ω_ℓ in each, and where the g.s. correlations have to be

known and used as input.

The e.s. equations (9) must again be truncated in practice, and again as the obvious extension of the g.s. SUBn scheme, I recall only the SUB(m,n) scheme where the operators $S^{(\ell)}_{m+i}$ and S_{n+i} are equated to zero for all $i \geq 1$, and the remaining n lowest g.s. Eqs. (5) and m lowest e.s. Eqs. (9) are solved together. There immediately arises at this point the problem of choosing "compatible" (m,n) pairs from the otherwise essentially distinct g.s. and e.s. CCF formalisms. With no further information, it is very difficult to know for example, whether increasing m for a <u>given</u> n (g.s. input) necessarily leads to increasingly "better" approximations. We shall see that the CCF linear response theory presented below can shed light on this question in its role as a bridge between the g.s. and e.s. formalisms.

3. LINEAR RESPONSE AND SUM RULES WITHIN THE CCF

As usual we now consider the response of the system in its g.s. to the addition of a small perturbation λv to the hamiltonian H, by expanding the g.s. energy and wavefunction in powers of the notional coupling parameter λ,

$$\begin{aligned} H \to H' &= H + \lambda v \ , \\ E \to E' &= E + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots \ , \\ |\Psi\rangle \to |\Psi'\rangle &= |\Psi\rangle + \lambda |\Psi^{(1)}\rangle + \lambda^2 |\Psi^{(2)}\rangle + \cdots \ . \end{aligned} \tag{10}$$

There are now various possible routes for a CCF analysis. Arponen,[11] for example, has defined $|\Psi'\rangle = \exp(S')|\Phi\rangle$ and used Eqs. (10) to determine the perturbed correlation operator S'. Guided by the usual derivation of sum rules however, we[1] have followed another route by making immediate contact with the excitation spectrum $|\Psi_\ell\rangle$ of the unperturbed hamiltonian H. We now restrict ourselves to first order changes in the g.s. wavefunction (<u>i.e.</u>, linear response) and expand $|\Psi^{(1)}\rangle$ as

$$|\Psi^{(1)}\rangle = \sum_\ell g_\ell |\Psi_\ell\rangle \ ; \quad H|\Psi_\ell\rangle = (E+\omega_\ell)|\Psi_\ell\rangle \ . \tag{11}$$

We further impose again the restrictions $\langle\Phi|\Psi_\ell\rangle = 0 = \langle\Psi|\Psi_\ell\rangle$ from the outset, for all states entering the assumed expansion (11), and we re-

strict ourselves also to perturbations v that satisfy the relations $\langle\Phi|v|\Psi\rangle = 0 = \langle\Psi|v|\Psi\rangle$, which are in fact satisfied by almost all perturbations of interest. Under these conditions, it is trivial to derive the usual results of (first- and second-order) perturbation theory that $E^{(1)} = 0$ and,

$$\sum_{\ell} \omega_{\ell} g_{\ell} |\Psi_{\ell}\rangle = -v|\Psi\rangle \quad ; \tag{12}$$

$$g_{\ell} = -\frac{1}{\omega_{\ell}} \frac{\langle\Psi_{\ell}|v|\Psi\rangle}{\langle\Psi_{\ell}|\Psi_{\ell}\rangle} \quad ; \tag{13}$$

$$E^{(2)} = \sum_{\ell} g_{\ell} \frac{\langle\Psi|v|\Psi_{\ell}\rangle}{\langle\Psi|\Psi\rangle} \quad . \tag{14}$$

By acting repeatedly on Eq. (12) with the operator (H-E), it is also easy to prove, for any positive integer m, the important relation,

$$\begin{aligned} &\sum_{\ell} \omega_{\ell}^{m} g_{\ell} |\Psi_{\ell}\rangle = -v_{(m)}|\Psi\rangle \quad ; \\ &v_{(1)} = v \; ; \; v_{(m)} = [H, v_{(m-1)}] \quad , \; m \geq 2 \quad . \end{aligned} \tag{15}$$

Equation (15) forms the basis for all of the ensuing sum rules, both for the well-known (various moments of the) energy-weighted dynamic liquid structure function $T(q,\omega)$ and, as we shall see, for their cluster decompositions.

3.1 CCF sub-sum-rules

Taking, for example, the inner product of Eq. (15) with the typical boson CCF states (5), after an initial pre-multiplication by e^{-S}, gives the double hierarchy of general sum rules (or, for reasons given below, what we shall call the CCF sub-sum-rules),

$$\sum_{\ell} \omega_{\ell}^{m} g_{\ell} S_{n}^{(\ell)}(\rho_1 \cdots \rho_n) = -\langle\Phi|(N^{-\frac{1}{2}} b_0^{\dagger})^n b_{\rho_n} \cdots b_{\rho_1} e^{-S} v_{(m)} e^{S}|\Phi\rangle \quad , \tag{16}$$

valid for arbitrary perturbation v. The sub-sum-rules (16) are now clearly seen to provide the bridge already mentioned between the excitation spectrum and its e.s. CCF description, which occur on the left-hand side only, and the g.s. CCF correlations which appear only on the right-hand side.

In order to make explicit further progress, we now specialize to

excited states which are eigenstates of momentum, and also restrict the remaining discussion to the very important illustrative example,

$$V \to \tfrac{1}{2}(\rho_{\vec{q}} + \rho^{\dagger}_{\vec{q}}) = V^{\dagger} \quad ; \quad q \neq 0 \quad ,$$
$$\rho_{\vec{q}} \equiv N^{-\frac{1}{2}} \sum_{\vec{k}} b^{\dagger}_{\vec{k}} b_{\vec{k}+\vec{q}} = \rho^{\dagger}_{-\vec{q}} \quad . \tag{17}$$

The operator $\rho^{\dagger}_{\vec{q}}$ creates a <u>density fluctuation</u> with momentum $\vec{q}$, and the perturbation (17) therefore destroys the translational invariance of the system. If we choose now to work in the natural momentum-eigenstate (<u>i.e.</u>, plane-wave) s.p. basis, and with the model state $|\Phi\rangle$ as the zero-momentum condensate, then Eq. (13) shows that the only excited states which carry non-zero weight g_{ℓ} in Eq. (11) are momentum eigenstates with eigenvalue $\pm\vec{q}$. Non-trivial results will thus be obtained from Eq. (16) only if the s.p. momenta $(\rho_1 \cdots \rho_n) \to (\vec{k}_1 \cdots \vec{k}_n)$ sum to $\pm\vec{q}$, and to be specific in the following discussion we shall assume they sum to $+\vec{q}$ (and hence that the excited states also have momentum eigenvalue $+\vec{q}$).

With this choice of perturbation from Eq. (17), the right-hand side of Eq. (16) can be evaluated explicitly for given indices (m,n). For example, the lowest three $n = 1$ sub-sum-rules can be evaluated as,

$$\sum_{\ell} \omega_{\ell} g_{\ell} S_1^{(\ell)}(q) = -\tfrac{1}{2}[1 + S_2(q)] \quad , \tag{18a}$$

$$\sum_{\ell} \omega_{\ell}^2 g_{\ell} S_1^{(\ell)}(q) = -\tfrac{1}{2} \frac{\hbar^2 q^2}{2m} [1 - S_2(q)] \quad , \tag{18b}$$

$$\sum_{\ell} \omega_{\ell}^3 g_{\ell} S_1^{(\ell)}(q) = -\tfrac{1}{2} \left\{ \left(\frac{\hbar^2 q^2}{2m} \right)^2 [1 + S_2(q)] - \frac{\hbar^2}{m} \sum_{\vec{q}'} (\vec{q}\cdot\vec{q}') V(q') \right. \tag{18c}$$
$$\left. \times \; [N^{\frac{1}{2}} S_3(\vec{q},\vec{q}',-\vec{q}-\vec{q}') + S_2(q') + S_2(\vec{q}+\vec{q}')] \right\} ,$$

where we have assumed again that the bosons interact only through pairwise forces with a local (velocity-independent) potential V, so that $[\rho_{\vec{q}}, V] = 0$. Given sufficient patience, similar sub-sum-rules can be evaluated for arbitrary (m,n).

3.2 Sum rules for the dynamic liquid structure function

We can also readily make contact with the usual sum rules for the energy-weighted moments of the dynamic liquid structure function $T(q,\omega)$,

$$T(q,\omega) \equiv \sum_\ell \frac{\langle\Psi|\rho_{\vec{q}}|\Psi_\ell\rangle\langle\Psi_\ell|\rho^\dagger_{\vec{q}}|\Psi\rangle}{\langle\Psi|\Psi\rangle\langle\Psi_\ell|\Psi_\ell\rangle}\,\delta(\omega-\omega_\ell) \quad , \tag{19}$$

by taking the inner product of our basic Eq. (15) with the state $v|\Psi\rangle$, and again restricting ourselves to perturbations v of the form (17). For example, the lowest two sum rules $(m = 1,2)$ are then easily shown to give the well-known "static sum rule" for the static structure function $T(q) \equiv \langle\Psi|\rho_{\vec{q}}\rho_{-\vec{q}}|\Psi\rangle / \langle\Psi|\Psi\rangle$, and the "f-sum rule"[12] respectively. Expressed in our CCF language and in the more usual way, these can respectively be written as,

$$2\sum_\ell \omega_\ell g_\ell \frac{\langle\Psi|\rho_{\vec{q}}|\Psi_\ell\rangle}{\langle\Psi|\Psi\rangle} = -T(q) \iff \int_0^\infty d\omega\, T(q,\omega) = T(q) \quad , \tag{20a}$$

$$2\sum_\ell \omega_\ell^2 g_\ell \frac{\langle\Psi|\rho_{\vec{q}}|\Psi_\ell\rangle}{\langle\Psi|\Psi\rangle} = -\frac{\hbar^2q^2}{2m} \iff \int_0^\infty d\omega\,\omega\, T(q,\omega) = \frac{\hbar^2q^2}{2m} \quad . \tag{20b}$$

Further information on these sum rules can be found, for example, in Refs. [13,14], and Feenberg[14] in particular also gives forms of the less well-known higher sum rules, with $m = 3,4$, in this hierarchy. Furthermore, in the limit of vanishing momentum transfer, the energy shift $E^{(2)}$ of Eq. (14) due to the perturbation (17) can also be calculated macroscopically in the usual well-known fashion,[13,14] to give the "compressibility sum rule",

$$\lim_{q\to 0} 2\sum_\ell g_\ell \frac{\langle\Psi|\rho_{\vec{q}}|\Psi_\ell\rangle}{\langle\Psi|\Psi\rangle} = -\frac{1}{2mc^2} \iff \lim_{q\to 0}\int_0^\infty \frac{d\omega}{\omega}\, T(q,\omega) = \frac{1}{2mc^2} \tag{21}$$

in terms of the (isothermal) first-sound velocity c.

In order to compare our sub-sum-rules (18a,b) with the sum rules (20a,b) it is convenient to expand $\langle\Psi|\rho_{\vec{q}}|\Psi_\ell\rangle \equiv \langle\Psi|e^{S}\mathbb{1}e^{-S}\rho_{\vec{q}}|\Psi_\ell\rangle$, by inserting for the unit operator $\mathbb{1}$ so indicated, the identity in the N-boson Hilbert space,

$$\mathbb{1} \equiv |\Phi\rangle\langle\Phi| + \sum_n \frac{1}{n!} \sum_{\rho_1 \cdots \rho_n} b^\dagger_{\rho_1} \cdots b^\dagger_{\rho_n} (N^{-\frac{1}{2}} b_0)^n |\Phi\rangle\langle\Phi| (N^{-\frac{1}{2}} b_0^\dagger)^n b_{\rho_n} \cdots b_{\rho_1} . \tag{22}$$

This then yields the expression,

$$\frac{\langle\Psi|\rho_{\vec{q}}|\Psi_\ell\rangle}{\langle\Psi|\Psi\rangle} = S_1^{(\ell)}(q) + \sum_{n=2}^{N} \frac{1}{n!} \sum_{\rho_1 \cdots \rho_n} \frac{\langle\Psi|b^\dagger_{\rho_1} \cdots b^\dagger_{\rho_n} (N^{-\frac{1}{2}} b_0)^n|\Psi\rangle}{\langle\Psi|\Psi\rangle} \times \langle\Phi|(N^{-\frac{1}{2}} b_0^\dagger)^n b_{\rho_n} \cdots b_{\rho_1} e^{-S_{\rho_{\vec{q}}}} |\Psi_\ell\rangle . \tag{23}$$

If Eq. (23) is now inserted into Eqs. (20), it is seen that the first term on the right-hand side of Eq. (23) thereby reproduces exactly the corresponding left-hand sides of Eqs. (18). From the remaining terms in Eq. (23), we get for $n > 1$, a very complex non-linear dependance on the g.s. subsystem amplitudes $\{S_n\}$, but with each term linear in the e.s. amplitudes $\{S_n^{(\ell)}\}$. We see in this way that the sets of sub-sum-rules (16) with $m = 1,2$ respectively and in each case for all n correspond just to Eqs. (20a) and (20b) respectively. In general we can see that [with the choice of perturbation of Eq. (17)] each sum rule from an energy-weighted moment (in index m) of the dynamic structure function is given a cluster decomposition (in index n) by our CCF sub-sum-rules (and hence this choice of name).

3.3 One-state approximation

Purely in order to demonstrate the sort of results obtainable with our new sub-sum-rules, we now make the drastic approximation that a single excited state ℓ exhausts the sum rules, which is the so-called one-state approximation. Simple division of the two lowest sub-sum-rules (18a) and (18b) then gives,

$$\omega \to \omega(q) = (\hbar^2 q^2/2m)[1 - S_2(q)]/[1 + S_2(q)] . \tag{24}$$

In order to make use of Eq. (21) in the interesting long-wavelength limit, we need now to approximate Eq. (23). In the spirit of the one-state approximation already made, the obvious choice is the RPA, which can be characterised in the present context by working in SUB2 approximation, with the further approximation of neglecting all contributions which depend on momenta other than $\pm\vec{q}$. In the RPA, only the term with

$n = 2$ survives out of the summand on the right-hand side of Eq. (23). A calculation within the RPA then shows,

$$\langle\Phi|(N^{-\frac{1}{2}}b_0^\dagger)^2 b_{\vec{q}} b_{-\vec{q}} e^{-S} \rho_{\vec{q}} e^{S} S^{(\ell)}|\Phi\rangle \simeq 2[1 + S_2(q)]S_1^{(\ell)}(q) \quad , \tag{25}$$

$$\langle\Psi|b_{\vec{q}}^\dagger b_{-\vec{q}}^\dagger (N^{-\frac{1}{2}}b_0)^2|\Psi\rangle / \langle\Psi|\Psi\rangle \simeq S_2(q) / [1 - S_2^2(q)] \quad , \tag{26}$$

where the symbol $\simeq$ indicates that these results are true only in the RPA. The derivation of Eq. (25) is straightforward, but the derivation of Eq. (26) requires a procedure similar to that used in deriving Eq. (23). Equation (21) thus reduces in the RPA to,

$$\lim_{q\to 0} \sum_{\ell} g_\ell S_1^{(\ell)}(q)[1 - S_2(q)]^{-1} \simeq -(4mc^2)^{-1} \quad . \tag{27}$$

Combining Eq. (27) with our previous Eqs. (18a,b), with all three evaluated in the one-state approximation, yields the further results,

$$\omega(q) \xrightarrow[q\to 0]{} \hbar c q \; ; \quad S_2(q) \xrightarrow[q\to 0]{} -1 + \frac{\hbar q}{mc} \quad . \tag{28}$$

Equation (28) shows how even this very simple approximation leads to the universal existence of a phonon spectrum in the long-wavelength limit. Furthermore substitution of Eq. (28) into the Bose equation for $S_2(q)$ in the RPA [obtained from Eq. (6b) by keeping only the first two out of the total of five terms on the left-hand side of Eq. (6b)] also yields precisely the well-known relationship for the first sound velocity,

$$c \simeq [NV(0)/m]^{\frac{1}{2}} \quad , \tag{29}$$

in the RPA. We note also that the static structure function can be similarly evaluated within the one-state approximation and the RPA from Eqs. (20a) and (18a) as,

$$T(q) \simeq [1 + S_2(q)] / [1 - S_2(q)] \quad . \tag{30}$$

Finally, a comparison of Eqs. (24) and (30) also yields the well-known Bijl-Feynman relation,

$$T(q)\omega(q) \simeq \hbar^2 q^2/(2m) \quad . \tag{31}$$

We note with interest that the only approximation involved in the derivation of Eq. (24) was the one-state approximation, whereas Eqs. (30) and (31) also require the RPA. However, we also note that making only the one-state approximation in Eq. (20b), which we have not yet

used, as well as in Eq. (20a) also immediately yields Eq. (31) directly, but now without use of the RPA. Thus an evaluation of $T(q)$ in an approximation other than RPA will clearly not be wholly compatible with the one-state approximation [at least as expressed by Eq. (31)]. Finally it is worth remarking that while the one-state approximation is wholly compatible with the RPA at the level of Eqs. (18a,b) and (20a,b) it is certainly not exact. When higher $(m > 2)$ $n = 1$ sub-sum-rules are considered, inconsistencies start to arise. (It is interesting to note however that Eq. (18c), for example, is also still compatible in the same one-state approximation with a long-wavelength phonon branch to the excitation spectrum, although now with a different expression for the velocity.)

4. CONCLUSIONS AND FINAL REMARKS

We have seen how to derive a set of exact sum rules within the CCF, which connect properties of the excitation spectrum (characterised by $|\Psi_\ell>$ and $S_n^{(\ell)}$) with ground-state correlations (characterised by $|\Psi>$ and S_n). This new double manifold (in moment index m and cluster-size index n) of sub-sum-rules (16) comprises a cluster decomposition (in index n) of each of the usual single manifold of sum rules for the m^{th} moments of the energy-weighted dynamic structure function, and hence can provide much more detailed information about many-body systems than the latter. The new formalism, suitably modified to deal with Fermi systems should be of particular use in the nuclear many-body problem, and where as a first step one might employ it to determine the g.s. correlation functions $S_n(q)$ for small clusters $n \gtrsim 2$, from experimental data on the excitation spectra. One could in this way try to use the wealth of information available on the excited states, to learn about the g.s. nuclear correlations which have otherwise proven so difficult to unravel. It is also quite likely, particularly within the context of the nuclear many-body problem, that our new sub-sum-rules will enable the CCF and the alternative moment methods[15] for nuclear many-body systems, to reinforce and illuminate one another, and perhaps to widen and strengthen their mutual field of applicability.

We have seen how even the simplest (one-state) approximation for the evaluation of our new sub-sum-rules leads to the important result of a phonon spectrum in the long-wavelength limit and also to the important Bijl-Feynman relation under the additional assumption of the RPA. We note that these results were derived using the (m,n) sub-sum-rules for the $n = 1$ clusters only. This is not too surprising since phonons may be quite accurately regarded as (collective) coherent superpositions of one-particle/one-hole excitations within the e.s. CCF. We also similarly expect that the same sub-sum-rules should be of value in the nuclear context in describing the "giant" collective resonances. Extensions of their use to the case $n > 1$ is also likely to be of some interest here.

An open question, of some considerable importance, remains how to improve upon the one-state approximation. However, the additional possible constraints of requiring arbitrarily many of the (m,n) sub-sum-rules to be compatible with each other (and perhaps with the corresponding sum rules for the dynamic structure function) should be of great value in the construction of improved approximations.

Finally, I would like to express the hope that the sum rule formalism developed here, may usher in a new round of applications of the CCF, which has hitherto largely been confined to (approximate solutions of) the g.s. and e.s. Schrödinger equation for a given many-body hamiltonian. At the very least, I am sure that the new formalism will prove useful in investigating the compatibility between the otherwise disconnected approximations used in the essentially distinct g.s. and e.s. CCF methods. On the wider front, I also believe that all nuclear systems to which the g.s. and e.s. CCF has already very successfully been applied,[7] might now profitably be subjected to further analysis with the tools of the sum rule formalism presented here.

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