Bishop

METHODS FOR THE MANY-BODY PROBLEM

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SOME RECENT DEVELOPMENTS IN COUPLED CLUSTER THEORY

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In this talk I intend to give a summary of work carried out in the last year or so at Manchester on developments of the coupled-cluster formalism of quantum many-body theory, and its application to infinite systems of bosons or fermions.

The usual starting-point for the coupled-cluster formalism is a re-expression of the many-body (ground-state) Schrödinger equation in terms of a set of non-linear coupled equations for the so-called correlation amplitudes. It is by now well known that the numerical solution of appropriate subsets of these equations has led to excellent quantitative results for systems as diverse as closed-shell atomic nuclei, the one-component Coulomb plasma, and even quite complex systems from the realm of quantum chemistry. More recently, Emrich has given a very elegant extension of the formalism to deal with excited states. In this talk I will describe how we have recently formulated linear response within the coupled-cluster framework, and have both used it to erect a bridge between the ground-state and excited-state theories, and have also thereby developed a very important and useful set of sum rules. I will then also describe their relationship to the usual well-known sum rules for the dynamic liquid structure function, $T(q,\omega)$. Any exact results in this field are clearly of considerable interest, and their derivation is one of the particular virtues of an exact microscopic theory. In this context, I shall show how our new hierarchies of sum rules constitute a decomposition of (the usual) sum rules for the structure function $T(q,\omega)$ into sub-sum-rules, and hence how they can provide much more detailed information about a many-body system than the structure function sum rules themselves can.

Purely for ease of exposition the discussion is given in terms of a many-boson system, for which the coupled-cluster Ansatz for the ground state (g.s.) eigenvector is given as

$$|\Psi\rangle = e^{S}|\Phi\rangle \quad ; \quad S = \sum_{n=2}^{\infty} S_n \quad , \tag{1}$$

in terms of a non-interacting zero-momentum condensate (model-ground state),

$$|\Phi\rangle = (N!)^{-\frac{1}{2}}(b_0^{\dagger})^N\,|0\rangle \quad . \tag{2}$$

The operator S_n excites n particle-hole pairs from this condensate

$$S_n = (n!)^{-1} \sum_{\rho_1 \cdots \rho_n} b^\dagger_{\rho_1} \cdots b^\dagger_{\rho_n} \, s_n(\rho_1 \cdots \rho_n) \, (N^{-\frac{1}{2}} b_0)^n \quad , \tag{3}$$

where the labels $\rho_1 \ldots \rho_n$ indicate non-zero single-particle momenta. The derivation of the coupled-cluster g.s. equations now proceeds in two simple steps. First the g.s. Schrödinger equation (with energy eigenvalue E) is multiplied by the operator exp(-S),

$$e^{-S} H e^{S} |\Phi\rangle = E |\Phi\rangle \quad , \tag{4}$$

which may be considered as a purely formal step to eliminate some "unlinked" terms from the outset that otherwise need to be eliminated later. Secondly, the scalar product of Eq. (4) is taken either with the state $|\Phi\rangle$ or the states

$$b^\dagger_{\rho_1} \cdots b^\dagger_{\rho_n} (N^{-\frac{1}{2}} b_0)^n \, |\Phi\rangle \tag{5}$$

When $\rho_1 \ldots \rho_n$ run over all momenta and when n runs from 2 to N, the vectors $|\Phi\rangle$ and (5) span the whole N-body Hilbert space (we can exclude $n = 1$, as in Eq. (1), from considerations of momentum conservation). The set of equations

$$\begin{aligned} &\langle\Phi| e^{-S} H e^{S} |\Phi\rangle = E \quad , \\ &\langle\Phi| (N^{-\frac{1}{2}} b_0^\dagger)^n \, b_{\rho_n} \cdots b_{\rho_1} \, e^{-S} H e^{S} |\Phi\rangle = 0 \quad , \end{aligned} \tag{6}$$

which are the g.s. coupled-cluster equations are hence fully equivalent to the original N-body Schrödinger equation.

Emrich has recently shown that for excited states $|\Psi_\ell\rangle$ which are orthogonal to $|\Phi\rangle$ and $|\Psi\rangle$, an appropriate choice of wavefunction is

$$|\Psi_\ell\rangle = S^{(\ell)} e^{S} |\Phi\rangle \quad ; \quad S^{(\ell)} = \sum_{n=1}^{\infty} S_n^{(\ell)} \quad ,$$

$$S_n^{(\ell)} = (n!)^{-1} \sum_{\rho_1 \cdots \rho_n} b^\dagger_{\rho_1} \cdots b^\dagger_{\rho_n} \, s_n^{(\ell)}(\rho_1 \cdots \rho_n) \, (N^{-\frac{1}{2}} b_0)^n \quad . \tag{7}$$

Each non-zero $S_n^{(\ell)}|\Phi\rangle$ is assumed to have a non-zero overlap with $|\Psi_\ell\rangle$. If the excited state is an eigenstate of momentum $\vec{q}$, this implies that the single-particle momenta $\rho_1 \ldots \rho_n$ in Eq. (7) must add to $\vec{q}$; whereas in the g.s. Eq. (3) they must add to zero. I shall also discuss an application of (both the g.s. and) Emrich's formalism to the problem of quasiparticle pairing in an infinite Fermi system, giving some exact results for a soluble model.

We now consider the response of the system to the addition of a small perturbation λv to the Hamiltonian H, by expanding the g.s. energy and wavefunction in powers of the coupling parameter λ,

$$H' = H + \lambda v \quad ,$$
$$E' = E + \lambda E^{(1)} + \lambda^2 E^{(2)} + \ldots \quad ,$$
$$|\Psi'\rangle = |\Psi\rangle + \lambda|\Psi^{(1)}\rangle + \lambda^2|\Psi^{(2)}\rangle + \ldots \quad . \tag{8}$$

One possibility to proceed further is now to define $e^{S'}|\Phi\rangle$ as the g.s. of H', and to use Eqs. (8) to determine S', as has recently been discussed by Arponen. Bearing in mind however the derivation of sum rules we wish to make contact with (some of) the excited states $|\Psi_\ell\rangle$ of H, and therefore make the Ansatz

$$|\Psi^{(1)}\rangle = \sum_\ell g_\ell|\Psi_\ell\rangle \quad ; \quad H|\Psi_\ell\rangle = E_\ell|\Psi_\ell\rangle \quad , \tag{9}$$

where the g_ℓ are unknown coefficients. We thus now restrict ourselves to first-order changes in the g.s. wavefunction (linear response theory). We impose as further restrictions that the $|\Psi_\ell\rangle$ entering Eq. (9) are orthogonal to $|\Phi\rangle$, and furthermore we choose the perturbation v such that the overlaps of $v|\Psi\rangle$ with $|\Phi\rangle$ and $|\Psi\rangle$ are both zero. Fairly standard linear response theory then leads to the first-order energy change vanishing, $E^{(1)} = 0$, and the results

$$\sum_\ell \omega_\ell\, g_\ell|\Psi\rangle = -v|\Psi\rangle \quad ; \tag{10}$$
$$g_k = -\frac{1}{\omega_k}\frac{\langle\Psi_k|v|\Psi\rangle}{\langle\Psi_k|\Psi_k\rangle} \quad ; \tag{11}$$
$$E^{(2)} = \sum_\ell g_\ell \frac{\langle\Psi|v|\Psi_\ell\rangle}{\langle\Psi|\Psi\rangle} \quad , \tag{12}$$

where we have introduced the notation $\omega_k \equiv E_k - E$. It is also straightforward to show that for any integral $m > 1$,

$$\sum_\ell \omega_\ell^m\, g_\ell|\Psi_\ell\rangle = -\,[H,[H,\ldots[H,v]\ldots]]|\Psi\rangle \quad , \tag{13}$$

where the nested commutator in Eq. (13) contains the Hamiltonian, H, (m-1) times.

Our particular hierarchies of coupled-cluster sum rules are now obtained from Eqs. (10) and (13) by taking their inner products with the states given in Eq. (5) after a first pre-multiplication by exp(-S), and by making use of the basic coupled-cluster Ansatzes of Eqs. (1)-(3) and (7). Equation (12) [which together with Eq. (11) is just second-order perturbation theory for the energy] may be regarded as a kind of zeroth-order sum rule. A particularly important application of the above analysis, motivated by the restrictions discussed after Eq. (9), follows from the choice

$$V = \frac{1}{2}\left(\rho_{\vec{q}} + \rho^{\dagger}_{\vec{q}}\right) \equiv V^{\dagger} \quad ; \qquad (q \neq 0) \quad , \tag{14}$$

$$\rho_{\vec{q}} \equiv N^{-\frac{1}{2}} \sum_{\vec{k}} b^{\dagger}_{\vec{k}}\, b_{\vec{k}+\vec{q}} \equiv \rho^{\dagger}_{-\vec{q}} \quad , \tag{15}$$

and I will discuss this in some detail. The operator $\rho^{\dagger}_{\vec{q}}$ creates a density fluctuation with momentum $\vec{q}$, and v thus destroys the translational invariance of the original H. The only excited states of interest [i.e., that carry non-zero weight g_{ℓ} in Eq. (9)] hence are momentum eigenstates with eigenvalue $\vec{q}$ or $-\vec{q}$, from Eq. (11). In this way, one can show, for example, that the lowest-order sum rules obtained as indicated above from Eqs. (10) and (13) [with m = 2], and using states (5) with n = 1, reduce to

$$\sum_{\ell} \omega_{\ell}\, g_{\ell}\, S_1^{(\ell)}(\vec{q}) = -\langle\Phi|\left(N^{-\frac{1}{2}} b^{\dagger}_{0}\right) b_{\vec{q}}\, e^{-S}\, v\, e^{S}|\Phi\rangle \equiv -F_1(\vec{q}) \quad ; \tag{16}$$

$$\sum_{\ell} \omega_{\ell}^2\, g_{\ell}\, S_1^{(\ell)}(\vec{q}) = -\frac{\hbar^2 q^2}{2m}\left\{1 - F_1(\vec{q})\right\} \quad . \tag{17}$$

In the limit of vanishing momentum transfer, the energy shift due to the perturbation of Eq. (14) can also be calculated macroscopically, in the usual well-known fashion, and gives the "compressibility sum rule" for the dynamic structure function, T(q,ω), which in our language can be expressed as

$$\lim_{q\to 0} 2\sum_{\ell} g_{\ell}\, \frac{\langle\Psi|\rho_{\vec{q}}|\Psi_{\ell}\rangle}{\langle\Psi|\Psi\rangle} = -\frac{1}{2mc^2} \iff \lim_{q\to 0} \int_0^{\infty} d\omega\, \omega^{-1}\, T(q,\omega) = \frac{1}{2mc^2} \tag{18}$$

in terms of the first-sound velocity, c. Two other well-known sum rules for T(q,ω), namely the "static sum rule" for the static structure function T(q) and the "f-sum rule" can also be rewritten in our fashion, and in the usual way for comparison, as

$$2\sum_{\ell} \omega_{\ell}\, g_{\ell}\, \frac{\langle\Psi|\rho_{\vec{q}}|\Psi_{\ell}\rangle}{\langle\Psi|\Psi\rangle} = -T(q) \iff \int_0^{\infty} d\omega\, T(q,\omega) = T(q) \quad ; \tag{19}$$

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

I show explicitly that our set of sum rules derived as described from Eq. (10) and the set of states (5) [for which Eq. (16) is the lowest ($n = 1$)] for $n = 1,2,\ldots$ corresponds precisely to Eq. (19). Similarly, the $m = 2$ sum rules derived from Eq. (13) [and see Eq. (17) for the $n = 1$ case] provide a decomposition (for $n = 1,2,\ldots$) of Eq. (20). The same is also true for (the perhaps less familiar) higher sum rules of the structure function (corresponding to $m \geq 3$).

Finally, as a very preliminary indication of the usefulness of the new sum rules, I show how by making the approximation of keeping only one state in the excitation spectrum, and applying the random-phase approximation in the low-momentum limit, one can "prove" (i.e., in this approximation) both the (universal) existence of a phonon spectrum in this limit, $q \to 0$, as well as the Bijl-Feynman formula relating the excitation spectrum and the static structure function. Although the one-state approximation is clearly not exact, we can undoubtedly use our sum rules to shed more light on these two simple (?), well-known, but very profound results of many-body theory. The difficulty of really proving that phonons become eigenstates in the limit as $q \to 0$ has been emphasised most strongly by Eugene Feenberg, and it is particularly gratifying to report here in St. Louis that a more detailed analysis, using the new sum rules, will almost certainly further clarify this important open problem stressed by him.