Chapter 3

The Coupled Cluster Method

We present here an overview of the CCM. For a more detailed exposition of the CCM, including a comprehensive list of references and a discussion of the treatment of excited states and dynamics in the CCM, see, *e.g.* [Bi91a], [Ar83a], or [Ar87]. A simple introduction to the CCM is also given in [Bi87].

The basic ingredients of the CCM are the so–called model state $|\Phi\rangle$, together with a set of mutually commuting (independent) multiconfigurational creation operators $\left\{C_I^\dagger\right\}$ defined with respect to the state $|\Phi\rangle$. The model state plays the role of a reference state or "vacuum", so that the state $C_I^\dagger|\Phi\rangle$ may be thought of as a multiparticle cluster configuration obtained by introducing I "elementary excitations" on $|\Phi\rangle$.

The CCM model state and corresponding creation operators must satisfy two essential requirements. Firstly, the state $|\Phi\rangle$ should not be orthogonal to the exact ground state. Thus one must ensure that the model state in-

corporates the underlying statistics and other symmetries of the many–body Hamiltonian. Furthermore, the creation operators $\left\{C_I^\dagger\right\}$ must be chosen such that the set $\left\{C_I^\dagger|\Phi\rangle\right\}$ spans the relevant many–body Hilbert space, *i.e.* such that $\left\{C_I^\dagger|\Phi\rangle\right\}$ is complete.

Besides these formal requirements, the choice of $|\Phi\rangle$ and $\left\{C_I^\dagger\right\}$ is in principle arbitrary [Bi91a]. It is clear that a judicious choice should lead to more rapid convergence of the CCM results, and this consideration should govern the choice of S and $|\Phi\rangle$. In practice, due to the complexity of the CCM calculations, the choice of the model state and cluster operator is often the simplest possible one satisfying the essential requirements listed above. There is no evidence in the literature that this choice has ever led to physically spurious predictions.

Although not essential, it is furthermore convenient for computational purposes if the creation operators are chosen such that

$$C_I|\Phi\rangle = 0 = \langle\Phi|C_I^\dagger \quad \forall \quad I \neq 0 \tag{3.1}$$

and

$$\langle\Phi|C_J C_I^\dagger|\Phi\rangle = 0 \quad \forall \quad J \neq I\,. \tag{3.2}$$

The first condition ensures that the Hermitian adjoint operators $\{C_I\}$ annihilate the model state, and the second that the states $\left\{C_I^\dagger|\Phi\rangle\right\}$ form a mutually orthogonal set. Unless stated otherwise, we will assume in what follows that this is the case.

To obtain a size–extensive result for the ground–state energy of a many–body system, the effective many–body Hamiltonian must be separable when

the system is separated into subsystems which are then removed sufficiently far from each other in configuration space (the so–called cluster property). In diagrammatic perturbation theory, Hugenholtz [Hu57, Tho] showed that linked (connected) diagrams always give contributions to the ground–state energy with the correct dependence on the extent of the system. Thus, in order to obtain results for the ground–state energy which obey the cluster property at any level of approximation, the energy must always be calculated as a sum over linked diagrams only. In the CCM, this is achieved by making the following ansatz for the ground–state wave function $|\Psi\rangle$:

$$|\Psi\rangle = e^S|\Phi\rangle \ , \qquad S = \sum_{I\neq 0} s_I C_I^\dagger \ . \tag{3.3}$$

The exclusion of the identity operator $C_0^\dagger \equiv 1$ from the cluster correlation operator S leads to the intermediate normalization condition

$$\langle\Phi|\Psi\rangle = \langle\Phi|\Phi\rangle = 1 \ , \tag{3.4}$$

provided that (3.1) is satisfied. The operator S, being additively separable, corresponds to a sum over linked diagrams, and therefore ensures the size–extensivity of the CCM ground–state energy at any level of approximation. The exponential form (3.3) also ensures the correct counting of all possible correlated I–body excitations from the model state.

In the CCM, the ground–state energy is now determined by rewriting the ground–state Schrödinger equation $H|\Psi\rangle = E_0|\Psi\rangle$ in the form

$$e^{-S}He^S|\Phi\rangle = E_0|\Phi\rangle \ . \tag{3.5}$$

The inner product of (3.5) with the model state $|\Phi\rangle$ yields

$$E_0 = \langle\Phi|e^{-S}He^S|\Phi\rangle \ , \tag{3.6}$$

which determines the ground–state energy E_0 as a function of the cluster correlation coefficients $\{s_I\}$. In turn, these coefficients are determined via the coupled equations

$$\langle\Phi|C_I e^{-S} H e^{S}|\Phi\rangle = 0\ , \tag{3.7}$$

obtained by taking the inner product of (3.5) with the set $\left\{C_I^{\dagger}|\Phi\rangle\right\}, I \neq 0$. The similarity transformed Hamiltonian $e^{-S}He^{S}$ can be expanded via the Hausdorff (nested commutator) expansion

$$e^{-S}He^{S} = H + [H,S] + \frac{1}{2!}[[H,S],S] + \ldots\ . \tag{3.8}$$

Provided that, as is the case for the model systems considered here, the many–body Hamiltonian contains a finite number of destruction operators defined with respect to the model state $|\Phi\rangle$, the nested commutator expansion (3.8) either terminates naturally at finite order or is resummable to closed form without approximation.

The CCM formalism as presented above, and in particular the ansatz (3.3) for the ground–state wave function, is in principle exact. However, in general the cluster correlation operator S must be summed to infinite order to obtain the exact solution. Therefore, in the application of the method, approximations are introduced since the operator S must be truncated in order to render the CCM equations (3.14) tractable. The truncation of S at finite order, say N, is referred to as the SUB-N approximation scheme, and has a physically intuitive and appealing meaning, namely that all I–body correlations on the model state $|\Phi\rangle$ up to $I = N$ have been included in the CCM approximation to the exact ground–state wave function. Although it is thus possible to systematically increase the order N of the SUB-N approxi-

mation scheme, there is however no guarantee that the corresponding results converge uniformly towards the exact results.

The determination of the ground–state expectation value $\overline{A}$ of an arbitrary operator A via the CCM requires, in addition to the CCM ground–state ket introduced above, also the ground–state bra. If the bra is simply taken as the Hermitian adjoint of the ket, then

$$\overline{A}_{\text{Hermitian}} = \frac{\langle\Phi|e^{S^\dagger}Ae^{S}|\Phi\rangle}{\langle\Phi|e^{S^\dagger}e^{S}|\Phi\rangle} = \langle\Phi|\left(e^{S^\dagger}Ae^{S}\right)_{\mathcal{L}}|\Phi\rangle \tag{3.9}$$

where the suffix $\mathcal{L}$ denotes a sum over linked diagrams. However, when expanded in powers of S and $S^\dagger$, the unitary (rather than similarity) transformed operator $e^{S^\dagger}Ae^{S}$ does not in general terminate after a finite number of terms, and it is not possible to write down an explicit expression for $\overline{A}_{\text{Hermitian}}$. Also, if the operators S and $S^\dagger$ are approximated by truncation at finite order, then $\overline{A}_{\text{Hermitian}}$ is no longer calculated from the same set of diagrams as for the energy [Tho], and therefore does not satisfy the requirements of the Hellmann–Feynman theorem [He35, Fe39].

For a system whose observables are represented by a set of Hermitian operators, the operators obtained via a similarity transform of the members of this set are in general non–Hermitian. It is always possible to regain a Hermitian description of the system, i.e. one where the observables have real eigenvalues and expectation values, via a redefinition of the scalar product (see also [Sc92]). For the reasons mentioned above, this is not done in the CCM. Rather, the ground–state bra $\langle\tilde{\Psi}|$ in the CCM is parameterized independently from the ket state $|\Psi\rangle$, and is thus not (to any finite order) the

manifest Hermitian conjugate of $|\Psi\rangle$ [1]. This non–Hermiticity can lead to imaginary values for the CCM energy, but, in earlier work, the appearance of an imaginary part in the energy has always correctly indicated a phase transition in the system (see e.g. [Ro90, Bi91b]). Also, as a result of the non–Hermiticity of the method, an approximate CCM result for the ground–state energy does not necessarily provide an upper bound for the true ground–state energy, despite the fact that, as will be shown shortly, the method may be formulated variationally. This loss of the upper–bound property is offset by the fact that the parameterization of the bra can be done in a manner which leads to explicit expressions for arbitrary expectation values, and which is compatible with the Hellmann–Feynman theorem at any level of approximation. Here we present two such formulations of the method [Ar83a]: In the so–called normal CCM (NCCM),

$$\langle\tilde{\Psi}|_{\rm NCCM} = \langle\Phi|\tilde{S}e^{-S}\ , \qquad \tilde{S} = 1 + \sum_{I\neq 0}\tilde{s}_I C_I\ , \tag{3.10}$$

whilst in the extended CCM (ECCM),

$$\langle\tilde{\Psi}|_{\rm ECCM} = \langle\Phi|e^{\Sigma}e^{-S}\ , \qquad \Sigma = \sum_{I\neq 0}\sigma_I C_I\ . \tag{3.11}$$

Here the bra–state coefficients $\{\tilde{s}_I\}$ ($\{\sigma_I\}$) are regarded as independent parameters; the Hermitian adjoint relation which formally specifies these parameters in terms of the ket–state coefficients $\{s_I\}$ is ignored. In both the NCCM and ECCM, condition (3.1) leads to the normalization

$$\langle\tilde{\Psi}|\Psi\rangle = \langle\Phi|\Phi\rangle = 1\ , \tag{3.12}$$

[1] To infinite order, the CCM prescription for the ground–state bra is formally identical to the Hermitian adjoint of the ground–state ket, and this non–Hermiticity disappears. In the application of the method, however, the cluster operator must in general be truncated for computational purposes, and this observation is thus mostly of academic interest.

and the expectation value of an arbitrary observable A is given by $\overline{A} \equiv \langle\tilde{\Psi}|A|\Psi\rangle$. In particular, the expectation value

$$\overline{H} \equiv \langle\tilde{\Psi}|H|\Psi\rangle \tag{3.13}$$

of the Hamiltonian becomes a functional of the NCCM (ECCM) coefficients $\{s_I, \tilde{s}_I\}$ ($\{s_I, \sigma_I\}$), which are then determined by the variational conditions

$$\frac{\partial\overline{H}}{\partial s_I} = 0 = \frac{\partial\overline{H}}{\partial\tilde{s}_I} \quad \left(\frac{\partial\overline{H}}{\partial s_I} = 0 = \frac{\partial\overline{H}}{\partial\sigma_I}\right) . \tag{3.14}$$

In both the NCCM and ECCM, the CCM ground–state energy is obtained by evaluating the energy functional $\overline{H}$ at the stationary point where the variational conditions (3.14) are satisfied. In the NCCM, the coefficients $\{\tilde{s}_I\}$ appear only linearly in the functional

$$\overline{H}_{\rm NCCM} = \langle\Phi|\tilde{S}e^{-S}He^{S}|\Phi\rangle , \tag{3.15}$$

so that the conditions

$$\frac{\partial\overline{H}}{\partial\tilde{s}_I} = \langle\Phi|C_I e^{-S}He^{S}|\Phi\rangle = 0 \tag{3.16}$$

identically reduce to the previous equations (3.7), and it is clear that the expression (3.6) for the CCM ground–state energy again obtains. Thus in the NCCM the coefficients $\{s_I\}$, and therefore also the CCM ground–state energy, are determined independently of $\{\tilde{s}_I\}$, and the bra–state coefficients are only required if other ground–state properties of the system are to be calculated. In the ECCM, however,

$$\overline{H}_{\rm ECCM} = \langle\Phi|e^{\Sigma}e^{-S}He^{S}|\Phi\rangle \tag{3.17}$$

and the CCM equations (3.14) for $\{s_I\}$ and $\{\sigma_I\}$ are coupled. Thus both sets of coefficients have to be solved for simultaneously in order to determine

the ground–state energy. As before, in the SUB-N approximation scheme, the operators $S, \tilde{S}$ (S, Σ) in the NCCM (ECCM) truncate at order N.

To any finite order in both the NCCM and ECCM, an arbitrary ground–state observable is calculated as a sum over linked diagrams only, and therefore exhibits the cluster property. In the NCCM, however, the ground–state bra amplitude $\tilde{S}$ itself contains unlinked terms. Due to its double exponential structure, the ECCM has the added advantage that both the ground–state ket and bra amplitudes are fully linked. As such, the ECCM, although computationally more involved than the NCCM, is capable of describing global phenomena such as phase transitions [Bi91a, Ar83a]. In the LMG model, for example, a spherical nucleus consisting of N nucleons undergoes a transition to a deformed shape above a region of critical coupling. The transition is only a true (sharp) phase transition in the thermodynamic limit $N \rightarrow \infty$ with the density of nucleons held fixed. Arponen [Ar82] has shown that, at least in low order (SUB-2), the NCCM based on a model state of spherical symmetry cannot accurately approximate the exact LMG ground–state energy in the deformed phase. Although no formal proof exists, it has been conjectured [Ar82] that the NCCM SUB-n results, for a model state of spherical symmetry, would not be accurate in the deformed phase for any finite n, and that a deformed model state is thus necessarily required for a successful NCCM calculation above the critical coupling regime. Subsequently, it was shown [Ar83a, Ar83b, Ro89] that it is possible, within the ECCM formulation of the method, to obtain accurate CCM results for the LMG ground–state energy over the full coupling spectrum, encompassing both the symmetric and deformed phases, using a single model state.