MAXIMUM ENTROPY VARIATIONAL APPROACH

TO COLLECTIVE STATES

N. Canosa, R. Rossignoli and A. Plastino

Departamento de Física, Universidad Nacional de La Plata
C.C. 67 (1900), La Plata, Argentina

Abstract

An approximation to the energy eigenstates of a many-body system, based on a previously introduced maximum entropy approach to the ground state, is developed and applied to a monopole fermion system. An excellent agreement with the exact eigenstates is obtained over the whole range of the pertinent coupling constant.

Introduction

The mean field method constitutes the basic approach to the many–fermion problem [1]–[3]. At the very least it yields the best zero–order wave function upon which to build up elementary excitations in order to describe low–lying excited states [2]. More recently, the maximum entropy principle derived from Information Theory (IT) [4]–[5] has proved to be a powerful tool to get insights into the complexity of the many–body problem. In a recent effort [6]–[10] an alternative, maximum entropy based approach to the description of many–body ground states has been introduced. By recourse to an appropiately defined *quantal* entropy that measures the lack of information concerning the probability distribution of a quantum state over an arbitrary basis, the method allows for a consistent theoretical picture of the ground state in terms of a small set of variables associated to relevant observables. It was shown that, just with a few one and two–body observables , diagonal in the given basis, this IT approximation yields ground state results in excellent agreement with the exact ones for a variety of many fermion models, for all values of the pertinent coupling constants, including transitional regions [6]–[10]. Here we wish to show how to build up elementary excitations upon such an IT based approximate ground state and, as an example, we tackle the description of the excited states of a many–body fermion model under a monopolar interaction.

The work is organized as follows: first, the IT approximation to the ground state is briefly reviewed followed by the extension of the formalism to excited states. Then, we illustrate our treatment with reference to an $SU(3)$ solvable model. Finally some conclusions are drawn.

Quantal Entropy and the Descrition of Ground States

We shall focus our attention upon systems described by a Hamiltonian of the form $\hat{H} = \hat{H}_0 + \hat{H}_{int}$, where $\hat{H}_0$ denotes the unperturbed term and $\hat{H}_{int}$ the corresponding interaction one. Let $\{\hat{O}_\alpha, \ \alpha = 1, \ldots, n\}$ be a set of relevant commuting operators that commute with $\hat{H}_0$ and which are thus diagonal in the appropriate common basis, in this case the unperturbed basis $\{|j\rangle, \ j = 1, \ldots, K\}$, formed by the eigenstates of $\hat{H}_0$. We shall consider a maximum entropy based exponential approximation [7, 8] to the ground state of the system, denoted by $|0\rangle$, of the form

$$|0\rangle = \sum_j C_j^{(0)} |j\rangle, \tag{1}$$

with

$$C_j^{(0)} = \exp\{-\tfrac{1}{2}[\lambda_0 + \sum_\alpha \lambda_\alpha O_\alpha(j)]\}, \tag{2}$$

where $O_\alpha(j) = \langle j|\hat{O}_\alpha|j\rangle$, $\{\lambda_\alpha = \lambda_\alpha^r + i\lambda_\alpha^i\}$ constitute a set of complex optimizable parameters and

$$\lambda_0 = \ln \sum_j \exp[-\sum_\alpha \lambda_\alpha^r O_\alpha(j)] \tag{3}$$

is the normalization constant (which can be taken as real). In this way the coefficients have the functional form typical of IT which *maximizes* the quantal entropy [6]–[7] in the common unperturbed basis, defined as

$$S = -\sum_j |C_j^{(0)}|^2 \ln |C_j^{(0)}|^2, \tag{4}$$

subject to the constraints

$$\langle \hat{O}_\alpha \rangle_0 \equiv \langle 0|\hat{O}_\alpha|0\rangle = O_\alpha. \tag{5}$$

We would like to remark here that the information entropy (4) is not the conventional thermodynamic one, which becomes zero for a pure state. The entropy (4) measures the lack of information concerning the probability distribution over the unperturbed basis, vanishing only in that special case in which $|0\rangle$ coincides with one of the eigenstates of $\hat{H}_0$. A smoothness criterium which is particularly suitable for ground states is obtained by means of the maximization of (4).

The formalism is able to yield both an *inference* scheme[7]–[8], in which the parameters λ_α are obtained according to the standard IT prescriptions, i.e. from the knowledge of the expectation values O_α (eqs. 5), and also can, alternatively, provide us with a pure *variational* treatment [7], [10]. The latter is the approach that we shall employ in this work. In the variational approximation the parameters λ_α result from the minimization of the ground state energy $\langle \hat{H} \rangle_0 = \langle 0|\hat{H}|0\rangle$, and in this case the appropriate relationships that define the set of general (complex) parameters λ_α are

$$-\partial \langle \hat{H} \rangle_0 / \partial \lambda_\alpha^r = \tfrac{1}{2} \langle \hat{O}_\alpha \hat{H} + \hat{H} \hat{O}_\alpha \rangle_0 - \langle \hat{O}_\alpha \rangle_0 \langle \hat{H} \rangle_0 = 0, \tag{6}$$

$$- \partial \langle \hat{H} \rangle_0 / \partial \lambda_\alpha^i = \tfrac{1}{2} \langle [\hat{H}, \hat{O}_\alpha] \rangle_0 = 0, \tag{7}$$

Eqs. (6) and (7) are together equivalent to the condition

$$\langle \hat{H} \hat{O}_\alpha \rangle = \langle \hat{O}_\alpha \hat{H} \rangle = \langle \hat{H} \rangle \langle \hat{O}_\alpha \rangle. \tag{8}$$

For the exact ground state, eqs. (6)–(7) are obviously satisfied for any operator $\hat{O}_\alpha$. Thus, it is apparent that convergence towards the exact ground state can be obtained by adding operators $\hat{O}_\alpha$ in the exponent of (2). The exact ground state coefficients can always be expanded in the form (2) if a complete set of diagonal operators $\hat{O}_\alpha$ is used [7].

If a prior estimate of the coefficients p_j is known, which can be either an approximate starting value or a multiplicity factor, i.e., a nonequal weight assigned to the unperturbed states the formalism can easily be extended to include this previous information. In this case one define the so called *surprisal* $I_j^2 = -\ln(|C_j^{(0)}|^2 p_j^2)$, (see for example Ref. [11]), so that the coefficients $C_j^{(0)}$ are now selected so as to maximize the *entropy defficienty*

$$\Delta S = \sum_j |C_j^{(0)}|^2 I_j^2, \tag{9}$$

i.e. the quantal entropy *relative* to the measure determined by p_j^2. The coefficients $C_j^{(0)}$ now acquire the appearance

$$C_j^{(0)} = p_j \exp\{-\tfrac{1}{2}[\lambda_0 + \sum_\alpha \lambda_\alpha O_\alpha(j)]\}. \tag{10}$$

The variational equations are obviously still given by (6)–(7). As we shall see, a good ansatz for the representation of excited states, which are characterized by the existence of nodes in the pertinent wave function, is available by recourse to suitable weight factors. This constitutes the central idea of the present work.

Quantal Entropy and Collective Excited States

We start the pertinent consideration by studying the states

$$|\alpha\rangle \equiv (\hat{O}_\alpha - \langle \hat{O}_\alpha \rangle_0)|0\rangle = \sum_j C_j^{(\alpha)}|j\rangle, \tag{11}$$

with

$$C_j^{(\alpha)} = C_j^{(0)}(O_\alpha(j) - \langle \hat{O}_\alpha \rangle_0) = -2\partial C_j^{(0)} / \partial \lambda_\alpha^r, \tag{12}$$

which can be regarded as maximum quantal entropy–defficienty coefficients. Here the prior knowledge entering the surprisal I_j is that provides by the measures $p_j = (O_\alpha(j) - \langle \hat{O}_\alpha \rangle_0)^2$. The states (11) are clearly *orthogonal* to the (approximate) ground state,

$$\langle 0|\alpha\rangle = 0 \tag{13}$$

and on account of the stability conditions (8), they verify,

$$\begin{aligned}
\langle 0|\hat{H}|\alpha\rangle &= \langle \hat{O}_\alpha \hat{H} \rangle_0 - \langle \hat{O}_\alpha \rangle_0 \langle \hat{H} \rangle_0 \\
&= 0.
\end{aligned} \tag{14}$$

Hence, the eqs. (6)–(7) imply that our approximate ground state is indeed stable against the excitations represented by the states $|\alpha\rangle$. This entails that for every operator included in the exponent of (2) there is no mixing between $|0\rangle$ and the states (11). Notice that these states are not orthogonal (and not normalized). For collective operators $\hat{O}_\alpha$, they can be regarded as furnishing a suitable basis for the description of collective excitations. As we can see, a first estimation of the low lying states can be obtained by diagonalizing $\hat{H}$ in this reduced space of dimension n. This can be accomplished by diagonalizing the pertinent overlap matrix, which coincides with the ground state covariance matrix,

$$\langle\alpha|\alpha'\rangle = \langle\hat{O}_\alpha\hat{O}_{\alpha'}\rangle_0 - \langle\hat{O}_\alpha\rangle_0\langle\hat{O}_{\alpha'}\rangle_0. \tag{15}$$

The hamiltonian matrix is of the form

$$\langle\alpha|\hat{H}|\alpha'\rangle = \langle\hat{O}_\alpha\hat{H}\hat{O}_{\alpha'}\rangle_0 - \langle\hat{O}_\alpha\rangle_0\langle\hat{O}_{\alpha'}\rangle_0\langle\hat{H}\rangle_0, \tag{16}$$

which is attained with the help of (8). The resulting approximate states can be cast as

$$|\beta\rangle \equiv (\hat{Q}_\beta - \langle\hat{Q}_\beta\rangle_0)|0\rangle, \tag{17}$$

where

$$\hat{Q}_\beta = \sum_\alpha b_{\alpha\beta}\hat{O}_\alpha, \tag{18}$$

and with the $b_{\alpha,\nu}$ arising from the eigenvector matrix of the system

$$hb = obh' \quad b^\dagger ob = I, \tag{19}$$

where o and h stand, respectively, for the overlap and hamiltonian matrices of elements (15) and (16), while $e_{\mu,\nu} = \delta_{\mu,\nu}E_\nu$ is the diagonal eigenvalue energy matrix. The orthogonal states (17) can thus be interpreted as *normal* modes.

In order to extend the formalism to higher excited states, we can construct in general the states

$$|\gamma\rangle \equiv (\prod_\alpha \hat{O}_\alpha^{n_\alpha} - \langle\prod_\alpha \hat{O}_\alpha^{n_\alpha}\rangle_0)|0\rangle, \tag{20}$$

where γ stands for $(n_1,\ldots,n_n)$, with $0 \leq n_\alpha \leq k_\alpha$, and diagonalize $\hat{H}$ in the ensuing reduced space. These states are in general not orthogonal, except with the approximate ground state ($\langle 0|\gamma\rangle = 0$), with an overlap matrix given by

$$\langle\gamma|\gamma'\rangle = \langle\prod_\alpha \hat{O}_\alpha^{n_\alpha+n'_\alpha}\rangle_0 - \langle\prod_\alpha \hat{O}_\alpha^{n_\alpha}\rangle_0\langle\prod_\alpha \hat{O}_{\alpha'}^{n_\alpha}\rangle_0. \tag{21}$$

In order to avoid superposition, we should obviously exclude from (20) those operators $\hat{O}_\alpha$ which can be expressed as products of other $\hat{O}'_\alpha$s. We could also employ the operators $\hat{Q}_\beta$ instead of $\hat{O}_\alpha$ in (20), reducing in this way the number of non-vanishing elements in the ensuing overlap and energy matrices. The space spanned by the states (20) is similar to that generated by the states $|\gamma'\rangle = \sum_j C_j'^{(\gamma)}|j\rangle$, with

$$C_j'^{(\gamma')} = \partial^k C_j^{(0)} / \prod_\alpha \partial\lambda_\alpha^{n_\alpha}, \tag{22}$$

where $k = \sum_\alpha n_\alpha$.

It is expected that a considerable part of the corresponding collective space will be spanned with low values of k_α, so that an accurate prediction of the low lying energy states can be achieved with a hamiltonian matrix $\langle \gamma | \hat{H} | \gamma' \rangle$ of small dimension and hence, the parameters λ_α can still be obtained *before* diagonalization by solving equations (6)–(7).

As we shall see in the next section our formalism is able to yield, in the example considered, a very accurate description of the lowest energy levels.

Application to a Monopole Model

In order to illustrate our formalism, we shall examine a $U(n)$ model [12]. We are dealing with $N = 2\Omega$ fermions distributed among $n = 2\Omega$–fold degenerate single particle (sp) levels with unperturbed energy ε_i coupled by a monopole interaction. The sp states are denoted as $|p, i\rangle$, $i = 1, \ldots, n$, $p = 1, \ldots, 2\Omega$. We shall consider the Hamiltonian

$$\hat{H} = \sum_i \varepsilon_i \hat{G}_{ii} - \tfrac{1}{2} \sum_{i<j} V_{ij}(\hat{G}_{ij}^2 + \hat{G}_{ji}^2), \tag{23}$$

where $\hat{G}_{ij} = \sum_p c_{pi}^\dagger c_{pj}$ are collective operators satisfying a $U(n)$ algebra under commutation. We shall take as expansion basis the eigenvectors of the unperturbed Hamiltonian $\sum_i \varepsilon_i \hat{G}_{ii}$ and shall consider $V_{ij} > 0$.

In the case $(N = 2\Omega)$ the ground state belongs to the completely symmetric representation $(N, 0, \ldots, 0)$ spanned by states $|m\rangle \equiv |m_1, \ldots, m_n\rangle$, $\sum_i m_i = N$, of dimension $\binom{N+2}{2}$, with m_i denoting the number of particles in the level i. The ground state $|\psi\rangle$ of (23) can be expanded as

$$|\psi_0\rangle = \sum_m C_m^0 |m\rangle, \tag{24}$$

where, due to the structure of this Hamiltonian, the sum can be restricted to states with even values of m_i, and all the ground state coefficients $C_m^{(0)}$ obviously possess the same phase.

We shall consider now the maximum quantal entropy approximation for the ground state (10). It has been shown that an excellent agreement with the exact ground state can be achieved employing just one and two–body diagonal operators in the exponent of the ground state coefficients, which amounts within the present context consider the operators $\hat{G}_{ii}$ and $\hat{G}_{ii}\hat{G}_{jj}$, $i \geq j > 1$. Thus, the ensuing approximate ground state coefficients are

$$C_m^{(0)} = p_m \exp[-\tfrac{1}{2}(\lambda_0 + \sum_{i>1} \lambda_i m_i + \sum_{i>j>1} \lambda_{ij} m_i m_j)], \tag{25}$$

with real λ_i and λ_{ij} determined by the set of equations (6)–(7). Here is interesting to remark that by setting $\lambda_{ij} = 0$ and employing a weight factor $p_m = N!/(\prod_i m_i!)$ in (25) we recover the *projected HF* coefficients [7]. Nevertheless, results with this factor and including $\lambda_{ij} \neq 0$ are of the same quality as those obtained from our maximum quantal entropy approximation [7] which, can obviously be obtained from (25) by setting $p_m = 1$.

Now let us turn our attention to the excited states of the symmetric representation. To this end we shall consider the approximate ground state (25) as a correlated vacuum

upon which we shall generate collective excitations. Following the previous section we construct first the states

$$|\psi_\gamma\rangle = [\langle \prod_i \hat{G}_{ii}^{n_i+n'_i}\rangle_0 - \langle \prod_i \hat{G}_{ii}^{n_i}\rangle_0 \langle \prod_i \hat{G}_{ii}^{n'_i}\rangle_0]|m\rangle \tag{26}$$

where the ensuing coefficients are given by

$$C_m^\gamma = C_m^{(0)}[\prod_{i>1} m_i^{n_i} - \langle \prod_{i>1} \hat{G}_{ii}^{n_i}\rangle_0] \tag{27}$$

with an overlap matrix

$$\langle \psi_\gamma | \psi_{\gamma'}\rangle = \langle \prod_i \hat{G}_{ii}^{n_i+n'_i}\rangle_0 - \langle \prod_i \hat{G}_{ii}^{n_i}\rangle_0 \langle \prod_i \hat{G}_{ii}^{n'_i}\rangle_0. \tag{28}$$

In this way the complete space correspond to the (projected) symmetric representation can be expanned, in the case $0 \leq m_i \leq k_i$ with $k_i = \binom{N+2}{2}$.

In order to construct the first excited states of the symmetric representation we shall consider the reduced basis formed by the states (25), with $0 \leq m_i \leq k_i$, and small decreasing values of k_i. In the case in which $0 \leq \sum_i m_i \leq 2$, we recover the states (11), the corresponding overlap and energy matrices (15)–(16) have the dimension $\binom{n+1}{2}$.

It is also possible to diagonalize first $\hat{H}$ in the space of dimension $n-1$ generated by the states

$$|i\rangle \equiv (\hat{G}_{ii} - \langle\hat{G}_{ii}\rangle)|0\rangle, \quad i \geq 2, \tag{29}$$

taking $\sum_i n_i = 1$ in (27), and then work with the *normal* operators (17)

$$\hat{G}'_{ii} = \sum_{j\geq 2} B_{ji}\hat{G}_{jj}, \tag{30}$$

with the matrix B determined by eqs. (19). We can construct higher excited states as in (27) employing the operators (30) instead of $\hat{G}_{ii}$.

As we shall see a very good agreement with the exact results can be obtained employing the previous formalism within the context of the present model. The figure is illustrative of the quality of the results obtained for the $SU(n)$ model with $n = 3$ (three–level case), for $N = 20$, $\varepsilon_i = (i-1)\varepsilon$ and $V_{ij} = (1 - \delta_{ij})v/(N-1)$. The three energy differences $\Delta E_i = E_i - E_0$; $i = 1, 2, 3$, corresponding to the four lowest lying levels of the pertinent energy spectrum are depicted. The approximate results were obtained after a 11×11 diagonalization in the reduced basis formed by states with coefficients (27). We note that in this model the HF approximation predicts second order ground state shape transitions in the classical limit ($N \to \infty$) with critical values at $v_{c1}/\varepsilon = 1$ and $v_{c2}/\varepsilon = 3$, corresponding to an spherical to deformed and to a deformed to deformed transitions [7]. Notice that the behaviour of the exact solution is obviously smooth for finite values of N, the same behaviour is obtained with our formalism. As we can see from the figure, our method is able to resolve even the tiny splitting between the second and the third excitation energies. The excellence of our approach is clearly appreciated, for the whole range of the coupling constant including transitional regions.

Conclusions

The present formalism provides one with a unified accurate description of the energy eigenstates, both in the low and strong coupling regimes, *including transitional* regions.

In a previous effort we had introduced a maximum quantal entropy approach which is able to yield an accurate description of the ground state of various fermion models in terms of a reduce set of variables associated with one and two-body relevant operators *diagonal* in a given unperturbed basis. In the present work we have extended the
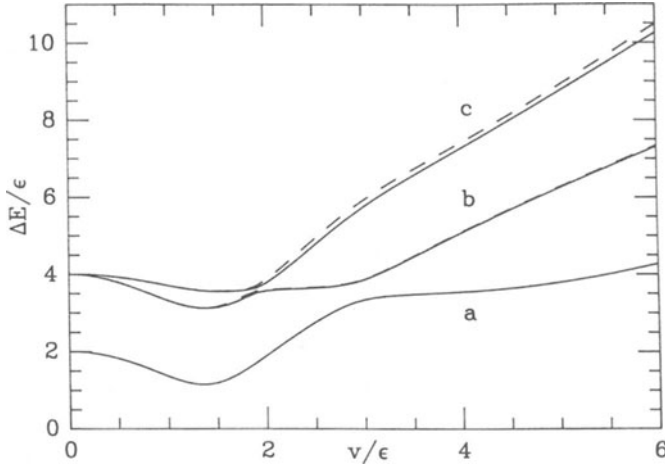
Figure 1. The first three excitation energies $\Delta E_i = E_i - E_0$, $i = 1, 2, 3$, curves (a), (b) and (c), respectively, corresponding to the four lying energy levels for $N = 20$ and $\varepsilon_i = (i-1)\varepsilon$ as a function of the coupling constant $V_{ij} = v/(N-1)$. Solid lines correspond to exact results and dashed lines to results obtained after a 11×11 diagonalization, indistinguishable in this scale.

scope of the previous general formalism in order to include the description of excited states. The approach provides a new simple scheme for generating collective excitations orthogonal to the maximum entropy ground state in terms of these diagonal operators.

In the example considered, results indicate that extremely accurate predictions of the lowest energy levels can be achieved in this way by means of the diagonalization of $\hat{H}$ in a basis of a quite *small* dimension. We can conclude that a new method for constructing general collective states on the basis of a suitably defined maximum quantal entropy correlated vacuum has been introduced.

Therefore, the present scheme may provide us with a useful way to generate collective spaces in many-body systems, in terms of a reduced set of variables. The excellent results should justify further works in more complex systems.

Acknowledgment

References

[1] D. J. Thouless, *The quantum mechanics of many body systems*, (Academic Press, New York, 1972).

[2] P. Ring and P.Schuck, *The nuclear many body problem*, (Springer, Berlin, 1980).

[3] A. de Shalit, H. Feshbach, *Theoretical nuclear physics*, (Wiley, New York, 1974).

[4] J. Jaynes, *Phys. Rev. 106 (1957) 620; 108 (1957) 171.*

[5] A. Katz, *Principles of statistical mechanics*, (Freeman, San Francisco, 1967).

[6] N. Canosa, A. Plastino and R. Rossignoli, *Phys. Rev. A 40 (1989) 519; Nucl. Phys. A 453 (1986) 457.*

[7] N. Canosa, R. Rossignoli and A. Plastino, *Nucl. Phys. A 512 (1990) 520.*

[8] N. Canosa, R. Rossignoli and A. Plastino *Phys. Rev. A 43 (1991) 1445.*

[9] N. Canosa, R. Rossignoli and A. Plastino, *Proceeding of Condensed Matter Theories XV (1992).* Ed. A. Protto and J. Aliaga (in press.)

[10] N. Canosa, A. Plastino, R. Rossignoli and H. G. Miller, *Phys. Rev. C 45 (1992) 1162.*

[11] J. Skilling, *Maximum Entropy and Bayesian Methods*, Kluwer Academic Publisher, Dordrecht, The Netherlands (1989).

[12] N. Meshkov, *Phys. Rev.C 3 (1971) 2214.*