The RPA correlation formula derived from the GCM/GOA

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time-odd extension by K. Matsuyanagi and T. Nakatsukasa (2005)

1. GCM/GOA

The small-amplitude limit of the Generator Coordinate Method in the Gaussian Overlap Approximation (GCM/GOA) is identical to RPA when the Hamiltonian is separable [1],[2]. In this note we go through the derivation, including the formula for the ground-state correlation energy, and extending the Hamiltonian to include a time-odd component.

The GCM states are denoted by $|q\rangle$. The necessary overlaps are parameterized in the GOA as

$$\langle q'|q\rangle = e^{-\alpha(q-q')^2}$$

$$\frac{\langle q'|H|q\rangle}{\langle q'|q\rangle} = h_0 - h_2(q-q')^2$$

where $h_{0,2}$ are functions of $\bar{q} = (q+q')/2$ only. We shall also restrict ourselves to the small amplitude limit about $q = 0$. Then except for an inconsequential constant term the Hamiltonian expression can be expanded as

$$\frac{\langle q'|H|q\rangle}{\langle q'|q\rangle} \approx \epsilon\bar{q}^2 - h_2(q-q')^2 \tag{1}$$

where now h_2 is a constant. With all these assumptions the system is harmonic. Thus, the ground state wave function will have the form

$$\Psi(q) = e^{-\beta q^2}.$$

All the needed integrals will be of the form

$$\langle\Psi|M|\Psi\rangle = \int dq \int dq' e^{-\beta(q^2+q'^2)}\langle q'|M|q\rangle$$

and since they are Gaussian integrals they are easy to do. The results are

$$\langle\Psi|\Psi\rangle = \frac{\pi}{\sqrt{2\beta\alpha+\beta^2}}$$

$$E \equiv \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\epsilon}{4\beta} - \frac{h_2}{2\alpha+\beta}.$$

We now minimize $E(\beta)$ with respect to β. The stationary condition $dE/d\beta = 0$ gives the condition

$$\frac{\alpha}{\beta} = \sqrt{\frac{h_2}{\epsilon}} - \frac{1}{2}. \tag{2}$$

This has a solution in the physically allowable domain ($\beta > 0$) provided

$$h_2 > \frac{\epsilon}{4}.$$

Otherwise, the best one can do is to take the state at $q = 0$ for the full wave function. Inserting the value of β at the minimum into the expression for the energy, we obtain the GCM/GOA result for the correlation energy,

$$E_0 = \frac{1}{2\alpha}(-\frac{\epsilon}{4} - h_2 + \sqrt{h_2\epsilon}) = -\frac{1}{2\alpha}\left(\frac{\sqrt{\epsilon}}{2} - \sqrt{h_2}\right)^2 \tag{3}$$

Now let us calculate the excitation energy. Assume the wave function to have the form

$$\Psi(q) = qe^{-\beta q^2},$$

and again minimize the expection value of the Hamiltonian with respect to β. The overlap is

$$\langle\Psi|\Psi\rangle = \frac{\pi}{\sqrt{2\beta\alpha + \beta^2}}\left(\frac{1}{4\beta} - \frac{1}{4(2\alpha+\beta)}\right).$$

The expection of the Hamiltonian is

$$\langle\Psi|H|\Psi\rangle = \frac{\pi}{\sqrt{2\beta\alpha + \beta^2}}\left(\frac{3\epsilon}{16\beta^2} - (\frac{\epsilon}{4} + h_2)\frac{1}{4\beta(2\alpha+\beta)} + \frac{3h_2}{4(2\alpha+\beta)^2}\right).$$

The ratio $r = \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ is minimized with respect to β using Mathematica, with a statement like

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Solve[D[r,b] ==0, b]
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The resulting β is the same as for the ground state , given by eq. (2). Substituting in the energy equation, we find

$$E_1 = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = -\frac{1}{8\alpha}(\epsilon - 12\sqrt{\epsilon h_2} + 4h_2).$$

The excitation energy is then given by

$$E_1 - E_0 = \frac{1}{\alpha}\sqrt{\epsilon h_2}. \tag{4}$$

2. RPA

We turn now to mean-field theory and RPA. We start with a mean-field ground state $|0\rangle$. Adding some external field to the Hamiltonian, there is a new mean-field state. We write the new state as

$$|q\rangle = N(q)\exp(qQ^\dagger)|0\rangle$$

where $Q^\dagger$ is some linear combination of particle-hole opeators $Q^\dagger = \sum_{ph} c_{ph} a_p^\dagger a_h$ and $N(q)$ is a normalization factor. We now make the boson approximation $[Q, Q^\dagger] = 1$ which allows one to calculate all the needed expection values. First, the normalization is found to be $N(q) = e^{-q^2}$. Next, the overlap

$$\langle q'|q\rangle = e^{-(q-q')^2/2}.$$

Thus, when we apply eq. (2), we will have $\alpha = 1/2$.

Now for the Hamiltonian. Taking a single ph state generated by $Q^\dagger$, the RPA Hamiltonian is simply the quadratic form,

$$H = \epsilon_{ph} Q^\dagger Q + \frac{v}{2}((Q^\dagger)^2 + Q^2) + vQ^\dagger Q \qquad (5)$$

The RPA equation is

$$\begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{pmatrix} Y \\ X \end{pmatrix} = \begin{bmatrix} \epsilon_{ph} + v & v \\ -v & -\epsilon_{ph} - v \end{bmatrix} \begin{pmatrix} Y \\ X \end{pmatrix} = \omega \begin{pmatrix} Y \\ X \end{pmatrix} \qquad (6)$$

Its eigenvalues are

$$\omega_{RPA} = \pm\sqrt{(\epsilon_{ph} + 2v)\epsilon_{ph}}. \qquad (7)$$

Now we find the GCM/GOA Hamiltonian corresponding to eq. (5). To evaluate matrix elements of H in the GCM states, it is convenient to use the identity

$$[Q, e^{qQ^\dagger}] = qe^{qQ^\dagger}.$$

It is then easy to show

$$\langle q'|Q^\dagger Q|q\rangle = q'q\langle q'|q\rangle$$

$$\langle q'|Q^2|q\rangle = q^2\langle q'|q\rangle,$$

etc. The Hamiltonian matrix elements are then

$$\frac{\langle q'|H|q\rangle}{\langle q'|q\rangle} = \epsilon_{ph} qq' + \frac{v}{2}(q^2 + q'^2) + vqq'.$$

Rewrite this in terms of $\bar{q}$ and $q - q'$: $qq' = \bar{q}^2 - (q-q')^2/4$ and $q^2 + q'^2 = 2\bar{q}^2 + (q-q')^2/2$. We then identify the terms in the GOA parameterization:

$$\epsilon = \epsilon_{ph} + 2v, \quad h_2 = \frac{\epsilon_{ph}}{4}.$$

In terms of the variables ϵ_{ph}, v, the condition for the existence of a nontrivial Ψ is simply $v < 0$ (only attractive interactions benefit from the GCM/GOA treatment).

Inserting the expressions for ϵ and h_2 in eq. (4), we find that the GCM/GOA excitation energy is equal to ω_{RPA}. The ground state energy in the GCM/GOA is

$$E = -\frac{1}{2}(\epsilon_{ph} + v) + \frac{1}{2}\sqrt{(\epsilon_{ph} + 2v)\epsilon_{ph}}.$$

This can be recognized as identical to the value obtained from RPA formula for the correlation energy,

$$E_{RPA} = \frac{1}{2}(\sum \omega_{RPA} - \mathrm{tr}A)$$

Finally, we ask, does the GCM/GOA still work when the interaction has a time-odd component? To address this question, let us generalize the Hamiltonian eq. (2a) by giving different strengths, v_1, v_2 to the two interaction terms,

$$H = \epsilon_{ph} Q^\dagger Q + \frac{v_1}{2}((Q^\dagger)^2 + Q^2) + v_2 Q^\dagger Q.$$

This introduces a time-odd component in the interaction given by $(v_1 - v_2)(Q^\dagger - Q)^2$. The RPA matrix becomes

$$\begin{bmatrix} \epsilon_{ph} + v_2 & v_1 \\ -v_1 & -\epsilon_{ph} - v_1 \end{bmatrix}$$

which has an eigenfrequency

$$\omega_{RPA} = \sqrt{(\epsilon_{ph} + v_1 + v_2)(\epsilon_{ph} + v_2 - v_1)}.$$

As before, we construct the GCM using only the time-even field $Q^\dagger + Q$. The Hamiltonian matrix element has the same form as before with the parameters ϵ and h_2 given by

$$\epsilon = \epsilon_{ph} + v_1 + v_2, h_2 = (\epsilon_{ph} + v2 - v1)/2.$$

Inserting this in eq. (4), we find the GOA excitation energy still agrees with the RPA value. Thus, a time-odd field does not seem to be needed in the GCM to generate the needed configurations for the RPA excitation energy.

[1] B. Jancovici and D.H. Schiff, Nucl. Phys. 58 (1964) 678.

[2] D.M. Brink and A. Weiguny, Nucl. Phys. A120 59 (1968).