The RPA correlation formula derived from the GCM/GOA


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

\[
\frac{\langle q'|H|q \rangle}{\langle q'|q \rangle} \approx \epsilon \bar{q}^2 - h_2(q - q')^2
\]

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

\[
\Psi(q) = e^{-\beta\bar{q}^2}.
\]

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 $\beta$. The stationary condition $dE/d\beta = 0$ gives the condition

$$\frac{\alpha}{\beta} = \sqrt{\frac{h_2}{\epsilon} - \frac{1}{2}}. \quad (2)$$

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 $\beta$ at the minimum into the expression for the energy, we obtain the GCM/GOA result for the correlation energy,

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

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

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

and again minimize the expectation value of the Hamiltonian with respect to $\beta$. 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 expectation of the Hamiltonian is

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

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

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Solve[D[r, b] == 0, b]
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The resulting $\beta$ 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

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

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

where $Q^\dagger$ is some linear combination of particle-hole operators $Q^\dagger = \sum_{ph} c_{ph} a^\dagger_{ph}$ 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 expectation 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,

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

(5)

The RPA equation is

$$\begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} Y \\ X \end{bmatrix} = \begin{bmatrix} \epsilon_{ph} + v & v \\ -v & -\epsilon_{ph} - v \end{bmatrix} \begin{bmatrix} Y \\ X \end{bmatrix} = \omega \begin{bmatrix} Y \\ X \end{bmatrix}$$

(6)

Its eigenvalues are

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

(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

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

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

$$\frac{\langle q'| H | q \rangle}{\langle q'| q \rangle} = \epsilon_{ph} q q' + \frac{v}{2} (q^2 + q'^2) + v q q'.$$
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 $\epsilon_{ph}, v$, the condition for the existence of a nontrivial $\Psi$ is simply $v < 0$ (only attractive interactions benefit from the GCM/GOA treatment).

Inserting the expressions for $\epsilon$ and $h_2$ in eq. (4), we find that the GCM/GOA excitation energy is equal to $\omega_{RPA}$. 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,

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

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,

$$H = \epsilon_{ph}Q^\dagger Q + \frac{v_1}{2}((Q^\dagger)^2 + Q^2) + v_2Q^\dagger Q.$$ 

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 $\epsilon$ and $h_2$ given by

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

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.