Utilizing Bogoliubov Transformations to Improve Accuracy in Computing Eigenvalues of Perturbed Harmonic Oscillators

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Many systems in physics can be modeled using harmonic oscillators, at a low approximation. Oscillations of larger amplitudes require higher-order approximations in order to accurately describe the motion of the system, so further investigation of anharmonicity becomes necessary. This project explores the analogue quantum mechanical system consisting of interacting particles subjected to forces which give rise to anharmonic oscillatory motion of the particles. In our case, this is done making use of diagrammatic, iterative, and computational techniques. Methods of improving accuracy and convergence for different energetic states are also developed and discussed.

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Introduction

- Quantum mechanical oscillations of a many-body system about a local potential minimum can in a first approximation be modeled by a set of harmonic oscillators about a local potential minimum. In this approximation the interaction potential of the system only retaining the lowest non-zero term in a Taylor expansion of the potential energy of the system around an equilibrium point, i.e. the term

$$\sum_{rs}\left(\frac{\partial^2 V}{\partial x_r x_s}\right)_{eq} x_r x_s$$

- The motion decouples into a system of independent quantum oscillators which can be compactly expressed in terms of bosonic creation and annihilation operators which create and annihilate vibrational quanta of modes with frequency ω_i respectively and the Hamiltonian takes on a very simple form

$$H_0 = \sum_{i=1}^{N}\left(a_i^\dagger a_i + \frac{1}{2}\right)\hbar\omega_i$$

- For a more detailed understanding it is typically necessary to include higher order terms in the Taylor expansion. In the *quartic* approximation, terms up to the fourth derivative of the potential energy are retained

$$\frac{1}{2!}\sum_{pq}\left(\frac{\partial^2 V}{\partial x_p \partial x_q}\right)_{eq} x_p x_q + \frac{1}{3!}\sum_{pqr}\left(\frac{\partial^3 V}{\partial x_p \partial x_q \partial x_r}\right)_{eq} x_p x_q x_r + \frac{1}{4!}\sum_{pqrs}\left(\frac{\partial^4 V}{\partial x_p \partial x_q \partial x_r \partial x_{rs}}\right)_{eq} x_p x_q x_r x_s$$

- The aim of our project is to develop a method to solve this *anharmonic* problem using coupled cluster techniques where terms beyond the harmonic approximation are treated as a perturbation.
- Here we present the first steps towards a systematic solution of ground and excited states of such a system using coupled cluster techniques applied to the resulting time-independent Schrödinger equation.

Equations of Motion-Coupled Cluster (EoM-CC) Approach

- We will first discuss the method we use in order to find the eigenvalues of this perturbed system. Everything in our derivation can be extended to include higher order terms if needed, though these terms would require extreme amounts of computational power to obtain in practice. The perturbing potential is assumed to be written in the following "normal ordered" form.

$$V_N = V_0 + V_1 + V_2 + V_3 + V_4 \qquad V_3 = \sum_{abc}\left(\frac{1}{3!}C_{abc}\,a_a^\dagger a_b^\dagger a_c^\dagger + \frac{1}{2!}K_{ab}^{c}\,a_a^\dagger a_b^\dagger a_c + \frac{1}{2!}K_{a}^{bc}\,a_a^\dagger a_b a_c + \frac{1}{3!}C^{abc}\,a_a a_b a_c\right)$$

- Our goal is to solve the resulting time-independent Schrödinger equation for *N* oscillators.

$$H\left|\psi\right\rangle = \left(H_0 + V\right)\left|\psi\right\rangle = \tilde{E}\left|\psi\right\rangle$$

- This is done by introducing a "cluster operator", consisting of all possible excitations of the system.

$$T = T_1 + T_2 + T_3 + \ldots = \sum_i t_i a_i^\dagger + \frac{1}{2!}\sum_{ij} t_{ij} a_i^\dagger a_j^\dagger + \frac{1}{3!}\sum_{ijk} t_{ijk} a_i^\dagger a_j^\dagger a_k^\dagger + \ldots \qquad \left|\tilde{0}\right\rangle = e^T\left|0\right\rangle$$

- With the new cluster operator, the Schrödinger equation for the perturbed ground state reads:

$$H\left|\tilde{0}\right\rangle = He^T\left|0\right\rangle = \tilde{E}_0 e^T\left|0\right\rangle \qquad \rightarrow \qquad e^{-T}He^T\left|0\right\rangle = \tilde{E}_0\left|0\right\rangle$$

- Via the use of the Baker-Campbell-Hausdorff formula, we can define an *effective* Hamiltonian.

$$\bar{H} = e^{-T}He^T = \left(He^T\right)_C \qquad \rightarrow \qquad \bar{H}\left|0\right\rangle = \tilde{E}_0\left|0\right\rangle$$

- Where the "C" subscript indicates that only contracted (or connected) terms are retained.
- The ground state energy and coupled cluster amplitudes can now be obtained from a set of coupled non-linear equations resulting from projections of the Schrödinger equation.

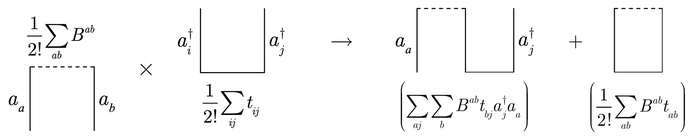
$$\left\langle 0\right|\bar{H}\left|0\right\rangle = \tilde{E}_0 \qquad \begin{aligned} t_i &: \quad \left\langle 0\right|a_i\bar{H}\left|0\right\rangle = 0 \\ t_{ij} &: \quad \left\langle 0\right|a_i a_j\bar{H}\left|0\right\rangle = 0 \end{aligned}$$

- In the EOM-CC method, excited states are obtained by diagonalizing the effective Hamiltonian matrix (which we note is no longer hermitean) in the basis of the *unperturbed* harmonic oscillator states. Symbolically, we can represent this by blocks involving the ground, first, second, etc. excited states.

$$\bar{\mathbf{H}} = \begin{pmatrix} \left\langle 0\right|\bar{H}\left|0\right\rangle & \left\langle 0\right|\bar{H}\left|1\right\rangle & \left\langle 0\right|\bar{H}\left|2\right\rangle & \cdots \\ \left\langle 1\right|\bar{H}\left|0\right\rangle & \left\langle 1\right|\bar{H}\left|1\right\rangle & \left\langle 1\right|\bar{H}\left|2\right\rangle & \cdots \\ \left\langle 2\right|\bar{H}\left|0\right\rangle & \left\langle 2\right|\bar{H}\left|1\right\rangle & \left\langle 2\right|\bar{H}\left|2\right\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Diagrammatics

- We can now express the Hamiltonian and the coupled cluster operator in diagrammatic form. By deriving diagrammatic rules, we can effectively calculate the necessary terms in our equations.
- As an example, the following diagrams illustrate how two operators can be connected in different ways, giving rise to two required terms in the EOM-CC operating equations.



- The resulting non-linear equations for the amplitudes are solved iteratively and a simple expression is found for the perturbed ground state energy. As the cluster operator includes infinitely many excitations, we require truncation at some point in order to solve the set of equations.
- For example, the ground state energy for a quartic perturbation including singly to quadruply excited amplitudes (T_1, T_2, T_3, T_4) is as follows.

$$\tilde{E}_0 = V_0 + \sum_a A^a t_a + \sum_{ab} B^{ab}\left(\frac{1}{2!}t_{ab} + \frac{1}{2!}t_a t_b\right) + \sum_{abc} C^{abc}\left(\frac{1}{3!}t_{abc} + \frac{1}{2!}t_{ab}t_c + \frac{1}{3!}t_a t_b t_c\right) +$$
$$+\sum_{abcd} D^{abcd}\left(\frac{1}{4!}t_{abcd} + \frac{1}{2!}\frac{1}{2!}t_{ab}t_{cd} + \frac{1}{3!}t_a t_{bcd} + \frac{1}{2!}\frac{1}{2!}t_a t_b t_{cd} + \frac{1}{4!}t_a t_b t_c t_d\right) + \frac{1}{2}\sum_a \omega_a$$

- Each individual matrix element in $\bar{H}$ can be calculated from similar equations, consisting of all possible diagrams with a certain string of operators.

Bogoliubov Transformations

- Noting that the above method is approximate, we can now utilize other techniques to greatly increase the accuracy of our result. Allow us, for example, to define a new set of creation and annihilation operators.

$$b_i^\dagger = \sum_j F_{ij} a_j^\dagger + \sum_j G_{ij} a_j + \sum_j D_{ij} \qquad \left[b_i, b_j^\dagger\right] = \delta_{ij} \qquad b_i\left|n\right\rangle_b = \sqrt{n}\left|n-1\right\rangle_b$$
$$b_i = \sum_j F_{ij}^* a_j + \sum_j G_{ij}^* a_j^\dagger + \sum_j D_{ij}^* \qquad\qquad b_i^\dagger\left|n\right\rangle_b = \sqrt{n+1}\left|n+1\right\rangle_b$$

- Utilizing the commutation relation and annihilation of the new ground state, we can show that the expansion coefficients defining the transformed operators are as follows for a single oscillator.

$$F = F^* = \left(1 - t_2^* t_2\right)^{-1/2}$$
$$D = -Ft_1^* = -\left(1 - t_2^* t_2\right)^{-1/2} t_1^*$$
$$G = -Ft_2^* = -\left(1 - t_2^* t_2\right)^{-1/2} t_2^*$$

- We can rewrite a general Hamiltonian which depends on the original operators in terms of the newly defined ones. This will give us a more accurate Hamiltonian to analyze using the coupled cluster method.

$$H_a = \frac{1}{2}\omega + \Delta a^\dagger a + \Lambda a^\dagger a^\dagger + \Lambda aa + \Gamma + \left(\alpha x + \beta x^2 + \gamma x^3 + \delta x^4\right)$$

$$H_b = \frac{1}{2}\omega + \Delta_b b^\dagger b + \Lambda_b b^\dagger b^\dagger + \Lambda_b bb + \Gamma_b + \left(\alpha_b x_b + \beta_b x_b^2 + \gamma_b x_b^3 + \delta_b x_b^4\right)$$

- Repeated Bogoliubov transformations of the above zeroth-order Hamiltonian will give us more and more accurate starting Hamiltonians. This is done iteratively via computer code.
- In order to connect these transformations to the coupled cluster approach, we simply need to use the proper initial conditions.

$$\Delta^{(0)} = \omega \quad ; \quad \Lambda^{(0)} = 0 \quad ; \quad \Gamma^{(0)} = 0$$

Conclusions and Future Work

We have presented example results for calculations of ground and excited state energies of a set of coupled oscillators using coupled cluster techniques. The process presented was illustrated for a quartic perturbation, for which an exact answer does not exist. Our next steps involve implementing the method in order to get numerical results for the case of multiple oscillators. Future work will include the application of the method to realistic physical systems, e.g. the case of anharmonic molecular vibrations where the necessary potential parameters can be obtained.

Quartic Perturbation of Single Oscillator

- The graphs below show the output from our Python code for the case of a single harmonic oscillator under quartic perturbation.
- The top graph – Examples of how the EoM-CC method compares to other methods of calculation for a pure quartic perturbation. Compared methods include numerical integration (which is exact) and different levels of perturbation theory (which are divergent for a quartic perturbation).
- The middle and bottom graphs – Comparison of results for excited state energies, calculated at three different stages (T=0, EoM-CC, and the fully converged result via Bogoliubov transformations) using 5x5 and 20x20 matrices.