جامعة الملك فهد للبترول والمعادن
King Fahd University of Petroleum & Minerals

Limitations of Perturbation Theory

PHYS410 Project

Ibraheem F. Al-Yousef
Department of Physics, KFUPM

Outline

Perturbation Theory

Definition

Perturbation Theory is a mathematical method used to solve problems which cannot be solved exactly. It involves breaking down a problem into a solved unperturbed part, then add a perturbation.

$$E_n = E_0 + \sum_{k=1}^{\infty} \lambda^k E_k$$

$$E_n^{(k)} = \frac{1}{k!} \frac{d^k E_n}{d\lambda^k}\bigg|_{\lambda=0}$$

$$\left|n^{(k)}\right\rangle = \frac{1}{k!} \frac{d^k |n\rangle}{d\lambda^k}\bigg|_{\lambda=0.}$$

Perturbation Theory Key Assumptions

- The perturbation is small relative to the unperturbed problem.
- The unperturbed problem is solvable easily. Exactly, or by an approximation. $H^0 |\psi^0\rangle = E^0 |\psi^0\rangle$
- The perturbation affects only a small part of the system: $V(x) \approx 0$ (for x outside the region where the perturbation is non-zero)

Main Areas of Usages

Remark

The principles of perturbation theory make it useful for usages in other fields and in different ways.

- Quantum Mechanics $\Longrightarrow$ Schrodinger's Equation.
- Quantum Field Theory $\Longrightarrow$ Scattering Amplitudes.
- Condensed Matter Theory $\Longrightarrow$ Physical Properties.
- Celestial Mechanics $\Longrightarrow$ Trajectories.
- Electrical Engineering $\Longrightarrow$ Circuits.
- More...

Main Areas of Usages

Remark

The main limitations of perturbation theory are inherited in the violations of its key assumptions.

- Divergence.
- Strong Perturbations.
- Unknown Unperturbed Solution.
- Non-adiabatic Systems.

Divergence in Perturbation Theory

Divergence Issue

In some cases, the series can diverge. This is called the divergence issue in perturbation theory, which is caused by the intricate relationship between the perturbation parameter and the physical parameters in the problem. Even though, the perturbed solution might be accurate in the physical regime where terms up to order n is sufficient, the convergence of the series might become slower and slower as the higher order terms are included.
The divergence of the perturbation series can be mitigated by introducing suitable renormalisation or transformation of the physical parameters.

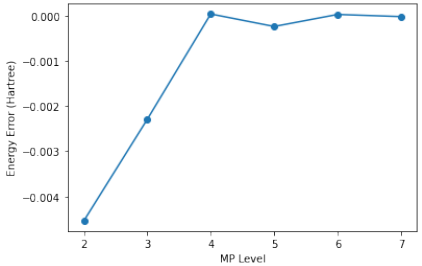
- Divergence occurs when the perturbative series does not converge, or when it converges to a value that is different from the exact solution.
- This can lead to inaccurate or unreliable results from perturbation theory, and it can limit the applicability of the method.

Examples: Møller–Plesset Perturbation Theory

Møller–Plesset perturbation theory

Møller–Plesset perturbation theory (MP) is one of several quantum chemistry post–Hartree–Fock ab initio methods in the field of computational chemistry. It improves on the Hartree–Fock method by adding electron correlation effects by means of Rayleigh–Schrödinger perturbation theory (RS-PT), usually to second (MP2), third (MP3) or fourth (MP4) order.

We can see that by adding higher order terms, we are not getting any advantage.



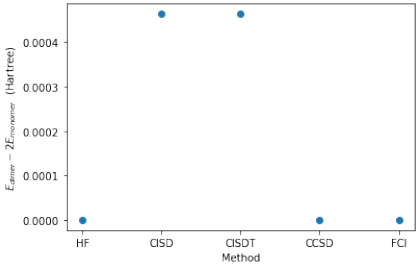
Examples: Coupled Cluster Theory

Coupled Cluster Theory

Coupled cluster (CC) is a numerical technique used for describing many-body systems. Its most common use is as one of several post-Hartree–Fock ab initio quantum chemistry methods in the field of computational chemistry, but it is also used in nuclear physics. Coupled cluster essentially takes the basic Hartree–Fock molecular orbital method and constructs multi-electron wavefunctions using the exponential cluster operator to account for electron correlation.

$$\Psi_{\mathrm{CCD}} = e^{\mathbf{T}}\Psi_{HF} = \left(1 + \mathbf{T}_2 + \frac{\mathbf{T}_2^2}{2!} + \frac{\mathbf{T}_2^3}{3!} + \cdots\right)\Psi_{HF}.$$

Coupled Clustered theory is one of the most successful post-Hartree–Fock ab initio quantum chemistry methods in the field of computational chemistry.



Conclusion: Perturbation Theory and its Limitations

- Perturbation theory is a powerful tool for solving problems in quantum mechanics.
- It allows us to approximate the solution of a complicated problem by breaking it down into simpler parts.
- However, it has its limitations. Such as the divergence, and the inability to treat strong perturbations.
- When perturbation theory fails due to divergence issues, it is often necessary to employ other techniques in order to solve the problem effectively.

Thank you!
Questions?