Quantum Many-Body Theory

Finding one and all roots to the couple cluster equations

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Introduction

- Newton's Method.
- Couple cluster equations.
- Homotopy.
- Bounding the number of roots

Couple cluster Ansatz I

CC is built on exponential Ansatz

$$\Psi = e^{T}\Phi_0$$

where ϕ_0 is the Hatree Fock state and $T(t) = \sum_{\mu} t_{\mu} X_{\mu}$ is defined by the excitation matrices. The eigenvalue problem becomes

$$\begin{aligned} H\Psi &= E\Psi \\ He^{T}\Phi_0 &= Ee^{T}\Phi_0 \\ e^{-T}He^{T}\Phi_0 &= E\Phi_0 \end{aligned}$$

For normalize Φ_0 this implies

$$\begin{cases} \langle \Phi_0, e^{-T}He^{T}\Phi_0 \rangle = E \\ \langle \Phi_{\mu}, e^{-T}He^{T}\Phi_0 \rangle = 0, \qquad \forall\, \Phi_{\mu} \perp \Phi_0 \end{cases}$$

We obtain a set of equations

$$\langle \Phi_{\mu}, e^{-T}He^{T}\Phi_0 \rangle = 0, \qquad \forall\, \mu \neq 0$$

Couple cluster Ansatz II

Recall that

$$T(t) = \sum_{\mu} t_\mu X_\mu.$$

This yields the couple cluster equations

$$f_\mu(t) = \langle \Phi_\mu, e^{-T(t)} H e^{T(t)} \Phi_0 \rangle = 0, \qquad \forall\, \mu \neq 0$$

The aim is ti find $\{t_\mu\}_{\mu \in I}$ such that $f_\mu(t) = 0 \qquad \forall\, \mu \in I$.

$$e^{-T(t)} H e^{T(t)} = H + [H, T] + 1/2[H, T]_2 + 1/6[H, T]_3 + 1/24[H, T]_4$$

where

$$[H, T]_n = [[[[H, T], T], \ldots], T]$$

Newton's Method

Suppose that $f : \mathbb{R} \to \mathbb{R}$ is a differentiable function with some unknown root $X_* \in \mathbb{R}$. Then

$$f(X_*) = 0.$$

- Root finding algorithm which produces successively better approximations to the roots of a real-valued function
- This method starts with an initial approximate root X_0 and constructs a sequence $X_0, X_1, X_2 \cdots$ of approximate roots.

Newton's Method in one variable

Suppose that we have an approximate root $x_0 \in \mathbb{R}$ that is close to x_*. From taylor series centered at x_0 we get

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0).$$

Put x_* into the taylor series to get

$$0 \approx f(x_0) + f'(x_0)(x_* - x_0)$$

Assuming $f'(x_0) \neq 0$ we have

$$x_* \approx x_0 - \frac{f(x_0)}{f'(x_0)}$$

This recursively gives

$$x_{k+1} \approx x_k - \frac{f(x_k)}{f'(x_k)}$$

Newton's Method in several variables

Suppose that we have an approximate root $\mathbf{X_0} \in \mathbb{R}^{\ltimes}$ that is close to $\mathbf{X}_*$. Then from the extension of the Newton method in one variable we get

$$\mathbf{X_{k+1}} \approx \mathbf{X_k} - \mathbf{F}'(\mathbf{X_k})^{-\mathbf{1}}\mathbf{F}(\mathbf{X_k})$$

where the jacobian $\mathbf{F}'(\mathbf{X_k})$ is invertible.

Observation on Newton's Method

- There are neighborhoods of the root inside which the Newton method will converge to the root.
- If it converges to the root then the convergence will be quadratic.
- At the boundary of the convergence area, the Newton method get stuck in a loop.

Example (Root finding)

- $f(x) = 4 + 8x^2 - x^4, \quad x_0 = 3$
- $f_1(x, y) = ye^x - 2,\ f_2(x, y) = x^2 + y^2 - 4, \quad X_0 = [-0.6, 3.7]^T$

The Root Structure of CC Theory

- In the context of CC methods, Newton-type methods are employed to approximate one root of the CC equations.
- From a computational perspective, (quasi) Newton-type methods have better numerical scaling than more general root-finding procedures.
- Additionally, in a perturbative regime, one could argue that the CC amplitudes can be viewed as minor corrections to the HF solution.

Newton Fractal I

consider the polynomial

$$p(z) = z^3 - 1$$

, whose roots are

$$z_1 = 1,\ z_{2,3} = -1/2 \pm i\sqrt{3}/2.$$

To find one root of the above system using Newton's method, we noticed that depending on the initial root, a different solution is found. This yields the known Newton fractal corresponding to p(z).
The white dots correspond to the roots z_1, z_2, z_3. The colored regions, red, blue, and green, correspond to the set of points that converges to the roots z_1, z_2, z_3 respectively. (Basin of attraction)

Newton Fractal II

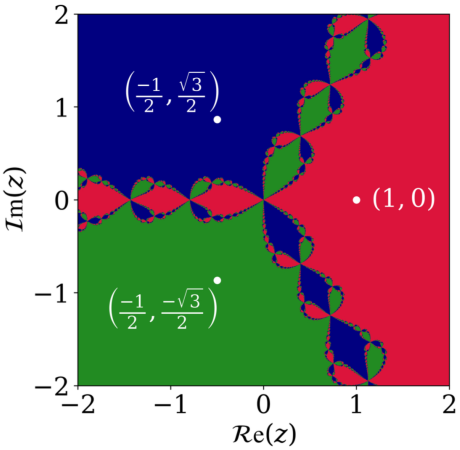

Figure: An example image

Homotopy Continuation I

This is to continuously transform a simple system of polynomials (auxiliary system) with known solutions into a more complex one (target system) and track the paths of these solutions. consider the couple cluster equation

$$F_{cc} = \begin{bmatrix} f_1(x_1, \cdots, x_m) \\ \vdots \\ f_m(x_1, \cdots, x_m) \end{bmatrix} = 0$$

idea:

- Construct an auxiliary system $G(X) = 0$ with known zeros and at least as many roots of F_{cc}.
- Define a family of systems $H(X, \lambda)$ for $\lambda \in [0, 1]$ interpolating between F_{cc} and G. i.e

$$H(X, 0) = F(X) \text{ and } H(X, 1) = G(X)$$

Homotopy Continuation II

- Track solutions along a path $X(\lambda)$ as we transition from $\lambda = 1$ to $\lambda = 0$. This procedure is equivalent to solving the IVP (Davidenko equation)

$$\frac{\partial}{\partial x} H(X, \lambda) \left(\frac{d}{d\lambda} X(\lambda) \right) + \frac{\partial}{\partial x} H(X, \lambda), \qquad X(1) = y_0$$

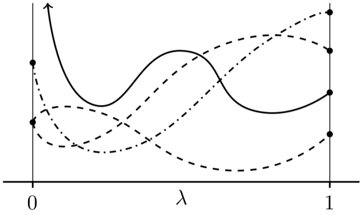

Figure: An example image

Homotopy Continuation III

Example (Homotopy)

Suppose we wish to solve $z^m = 0$. Using homotopy

$$\lambda(z^m - 1) + (1 - \lambda)z^m = 0.$$

When $\lambda = 1$, we start with roots of unity. i.e

$$z^m = 1 \quad \rightarrow z_k = \exp(2\pi ik/n) \quad k = 0, 1, \dots, m-1$$

As $\lambda \rightarrow 0$ we get

$$z^m = \lambda$$

$$z^j(\lambda) = \mu^j \sqrt[m]{\lambda}$$

where μ^j is primitive root of unity. Hence the solution to $z^m = 0$ are paths given for any particular value of λ by

$$z^j(\lambda) = \exp(2\pi ij/n) \sqrt[m]{\lambda}$$

Number of roots - The Bézout bound I

A good estimate for the number of roots is needed!

- Product of the degrees of the individual polynomials is an upper bound to the number of roots
- A drawback of Bézout's Theorem is that it yields little information for polynomials that are sparse!

Example

$f(x, y) = a_1 + a_2 x + a_3 xy + a_4 y$ and $h(x, y) = b_1 + b_2 x^2 y + b_3 xy^2$
with generic choices of coefficients a_i and b_j.
$\Rightarrow$ Four distinct roots
Bézout bound: $\deg(f) \cdot \deg(h) = 2 \cdot 3 = 6$

Number of roots - Bernstein-Khovanskii-Kushnirenko

Consider

$$\begin{aligned} f(x,y) &= a_1 + a_2x + a_3xy + a_4y \\ &= a_1x^0y^0 + a_2x^1y^0 + a_3x^1y^1 + a_4x^0y^1 \end{aligned}$$

This yields

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

which yields the Newton polytope $\mathrm{New}(f) =: P$

Number of roots - Bernstein-Khovanskii-Kushnirenko

Similarly

$$h(x, y) = b_1 + b_2x^2y + b_3xy^2$$

This yields

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

which yields the Newton polytope $\text{New}(h) =: Q$

Number of roots - Bernstein-Khovanskii-Kushnirenko

BKK-Theorem (bivariant polynomials):
If f and h are two generic bivariate polynomials, then the number of solutions of $g(x, y) = h(x, y) = 0$ in $\mathbb{C}^2$ equals the mixed area

$$\mathcal{M}(\mathrm{New}(f), \mathrm{New}(h))$$

where

$$\mathcal{M}(P, Q) = \mathrm{area}(P \oplus Q) - \mathrm{area}(P) - \mathrm{area}(Q)$$

and

$$P \oplus Q = \{p + q \mid p \in P, q \in Q\}$$

is the Minkowski sum.