Resummation of divergent series via analytic continuation

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Application of the Cauchy integral formula as a tool of analytic continuation for the resummation of divergent perturbation series

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Analytic-continuation approach to the resummation of divergent series in Rayleigh-Schrödinger perturbation theory

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Let us assume the non-Hermitian eigenvalue problem

$$\hat{H}(z)\Psi(z) = (\hat{H}^{(0)} + z\hat{V})\Psi(z) = E(z)\Psi(z)$$

where z is a complex perturbation parameter that one sets to $z = 1$ for the physical system

One can expand the energy as a power series following Rayleigh-Schrödinger perturbation theory

$$E(z) = \sum_{k=0}^{\infty} z^k E^{(k)}$$

This series is convergent for $|z| < |z_0|$ where $|z_0|$ is the radius of convergence

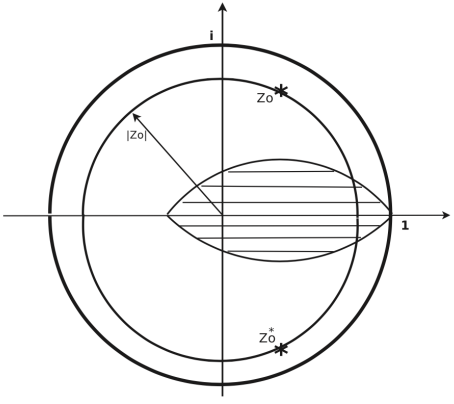


FIG. 1. Schematic contours on the complex plane exhibiting the (outer) unit circle, the location of the closest singularities z_0, z_0^*, the convergence radius $|z_0|$, the domain of convergence (inner circle), and an area bordered by an artificial contour to be used for the application of the Cauchy integral formula (shaded domain).

Let us consider the divergent series

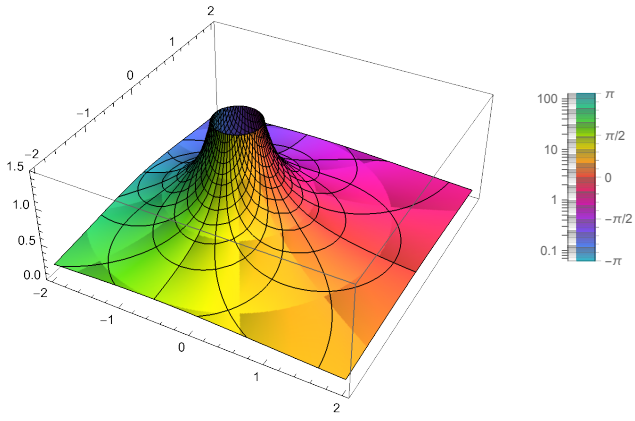
$$f(1) = \sum_{k=0}^{\infty} (-2)^k = 1 - 2 + 4 - 8 + 16 - 32 + \cdots$$

which can be generalized as

$$f(z) = \sum_{k=0}^{\infty} (-2)^k z^k = \frac{1}{1+2z}$$

$f(z)$ is convergent for $|z| < 1/2$ but $f(1) = 1/3$!!

Simple example of analytic continuation



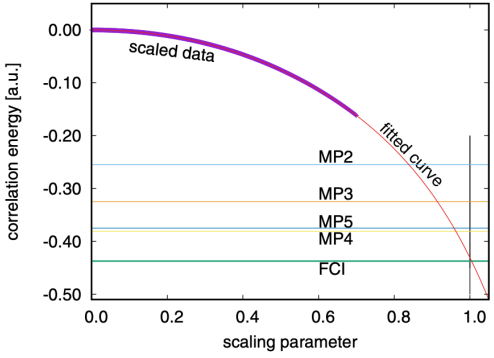


FIG. 4. Analytic continuation of the scaled sums of perturbative corrections for the correlation energy of the water molecule. The horizontal levels marked "MPn" indicate the energies of the PT series at order n. Dense purple dots indicate the scaled sums, continued by the red solid curve by polynomial fitting. The green horizontal line "FCI" indicates the correlation energy as obtained by exact diagonalization with the two core ($1s$) electrons kept frozen.

Theorem

Let U be an open subset of the complex plane $\mathbb{C}$, and suppose the closed disk D defined as

$$D = \{z : |z - z_0| \leq r\}$$

is completely contained in U. Let $f : U \to \mathbb{C}$ be a holomorphic function, and let γ be the circle, oriented counterclockwise, forming the boundary of D.
Then for every a in the interior of D,

$$\boxed{f(a) = \frac{1}{2\pi i} \oint_\gamma \frac{f(z)}{z - a} dz}$$

1. Compute as many terms as possible: $E^{(0)}$, $E^{(1)}$, $E^{(2)}$, $E^{(3)}$, etc and estimate the radius of convergence
2. Pick a contour that goes through $z = 1$ and encloses points of the "trusted region". No singularities inside the contour to ensure $E(z)$ is analytic inside.
3. Evaluate $E(z)$ on the contour inside the trusted region.
4. Pick a values inside the trusted region and evaluate $E(a)$ via the truncated series.
5. Use these values to estimate $E(z)$ on the contour outside the trusted region including $E(z = 1)$
6. Compute $E(a)$ for the points inside the trusted region via Cauchy's integral formula. The difference with the previous values is an estimate of the error
7. Modify the values on the contour to minimize error and iterate.
8. When converged, $E(z = 1)$ is an estimate of the FCI energy!

TABLE I. Correlation energy of the LiH molecule at several geometries and at various orders of MP PT and their resummed value. Energies are in mE_h. (For the meaning of r_0, see the text.)

$R_{Li-H}/Å$	r_0	E_{MP5}	E_{MP6}	E_{FCI}	E_{Cauchy}
0.9	0.7	−51.680	−51.868	−51.968	−51.965
1.0	0.7	−50.433	−50.602	−50.690	−50.688
1.1	0.7	−49.302	−49.459	−49.542	−49.539
1.2	0.7	−48.317	−48.468	−48.550	−48.548
1.3	0.7	−47.485	−47.634	−47.721	−47.718
1.4	0.7	−46.800	−46.952	−47.049	−47.045
1.5	0.7	−46.258	−46.420	−46.532	−46.527
1.6	0.7	−45.857	−46.034	−46.170	−46.164
1.7	0.7	−45.594	−45.794	−45.961	−45.955
1.8	0.7	−45.464	−45.694	−45.905	−45.896
1.9	0.7	−45.459	−45.727	−45.994	−45.983
2.0	0.7	−45.570	−45.884	−46.225	−46.209
2.5	0.7	−47.611	−48.300	−49.393	−49.332
3.0	0.7	−51.760	−53.152	−56.111	−55.982
3.5	0.7	−57.978	−60.651	−66.860	−67.094
3.75	0.95	−62.019	−65.713	−73.498	−73.499
4.0	0.94	−66.842	−71.966	−80.532	−80.491
4.5	0.86	−79.382	−89.369	−94.401	−93.660

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