Nonlinear Eigenvalue Algorithms with Applications

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Eigenvalue problems in which the coefficient matrices depend nonlinearly on the eigenvalues arise in a large variety of applications. Eigenvalues λ associated with eigenvectors $\mathbf{x}$ are then solutions of the following general form:

$$\mathbf{T}(\lambda)\mathbf{x} = 0. \tag{1}$$

This formulation includes the common linear eigenvalue problem as a special case, letting
$\mathbf{T}(z) = z\mathbf{B} - \mathbf{A}$,
as well as the polynomial case letting
$\mathbf{T}(z) = \sum_{m=0}^{M} z^m \mathbf{A}_m$.
Most often, however, numerical modeling of physical systems gives rise to the following non-linear eigenvalue form:

$$\mathbf{T}(z) = z\mathbf{S} - (\mathbf{H} + \mathbf{\Sigma}(z)), \tag{2}$$

where $\mathbf{H}$ represents the Hamiltonian, $\mathbf{S}$ is the mass matrix (i.e. $\mathbf{S} = \mathbf{I}$ using orthogonal basis functions), and $\mathbf{\Sigma}$ is a non-linear matrix with z. We note that $\mathbf{T}(z)^{-1}$ is the Green's function $\mathbf{G}(z)$ of the system. Depending on the applications, $\mathbf{\Sigma}$ has different meaning, for example:

- In quantum transport modeling (NEGF), $\mathbf{\Sigma}$ represents the self-energy functions that guarantee transparent/open/absorbing boundary conditions with the contact reservoirs.
- In electronic structure GW modeling, $\mathbf{\Sigma}$ represents the exact exchange and correlations terms that must be including to accurately predict bandgaps of materials in many-body perturbation theory (we note that only the correlation part is non-linear).
- In domain decomposition approach, $\mathbf{\Sigma}$ may represent a Schur complement arising while attempting to express a linear eigenvalue problems into a reduced system size (including the notable example of the Slater APW approach).

A common strategy for addressing these problems is linearization, which approximates the term $\mathbf{\Sigma}(z)$. However, this approach can introduce errors that compromise accuracy. Moreover, linearization often leads to larger systems and may necessitate the use of less robust numerical methods, such as the graphical or spectral method for GW. Our goal is to enable the direct solution of the non-linear problem (2) in a way that is: (i) robust, requiring no approximations; (ii) broadly applicable, with a general approach independent of the specific form of the non-linearity; and (iii) efficient, ensuring numerical scalability and high performance. This is made possible by enhancing the FEAST eigenvalue algorithm to naturally incorporate non-linear effects. FEAST reformulates the eigenvalue problem into a series of independent linear system solves at specific contour points. Using contour integration along $\mathbf{\Gamma}$, it iteratively refines the solution space via inversion residual subspace iterations. The nonlinear FEAST algorithm involves performing the following contour integrations along Γ for $k = 0$ and $k = 1$:

$$\mathbf{Q}_k = \frac{1}{2\pi\imath} \oint_{\Gamma} z^k \Big(\mathbf{X} - \mathbf{T}^{-1}(z)\mathbf{R}\Big)(z\mathbf{I} - \mathbf{\Lambda})^{-1}\, dz. \tag{3}$$

Using $\mathbf{Q}_k$, one can construct a reduced eigenvalue problem using Rayleigh–Ritz method [1], [2], [3].

We apply this new nonlinear eigenvalue algorithm to address the three problems described above. Our findings outlines, in particular, the importance of considering nonlinear eigenvalue problems in GW approximations to accurately obtain both HOMO and LUMO states.

References

[1] B. Gavin, A. Miedlar and E. Polizzi, Journal of Computational Science 27, 107, (2018).
[2] J. Brenneck and E. Polizzi, arXiv:2007.03000, (2020).
[3] D. Li and E. Polizzi, Phys.Rev. B 111 (4), 045137, (2025).

	Molecule	G_0W_0@PBE Graphical solution	Spectral functions	Nonlinear FEAST	Deviation
	He	−23.66	−23.69	−23.69	0.03
	H_2	−15.91	−15.92	−15.92	0.01
	Ne	−20.75	−20.78	−20.78	0.03
HOMO	LiH	−6.94	−6.97	−6.97	0.03
	Li_2	−5.05	−5.02	−5.02	−0.03
	CO	−14.08	−14.09	−14.09	0.01
	F_2	−15.03	−15.07	−15.07	0.04
	He	2.06	1.91	1.91	0.15
	H_2	2.57	1.95	1.95	0.62
	Ne	2.45	2.16	2.16	0.29
LUMO	LiH	0.47	0.32	0.32	0.15
	Li_2	−0.03	−0.09	−0.09	0.06
	CO	0.35	0.21	0.21	0.14
	F_2	−1.40	−1.59	−1.59	0.19

Fig. 1: Nonlinear FEAST G_0W_0 results using Kohn-Sham PBE as the starting point, compared to conventional methods (spectral functions and graphical solutions), HOMO and LUMO energies in eV (Extracted from [3])

Fig. 2: All scattering resonances from a quantum transport problem. The nonlinear FEAST scheme is using a search subspace size of $m_0 = 30$ to capture all of the 22 eigenvalues inside of the integration contour, plus the eight (8) eigenvalues that are closest to the integration contour while still being outside of it. (Extracted from [1])

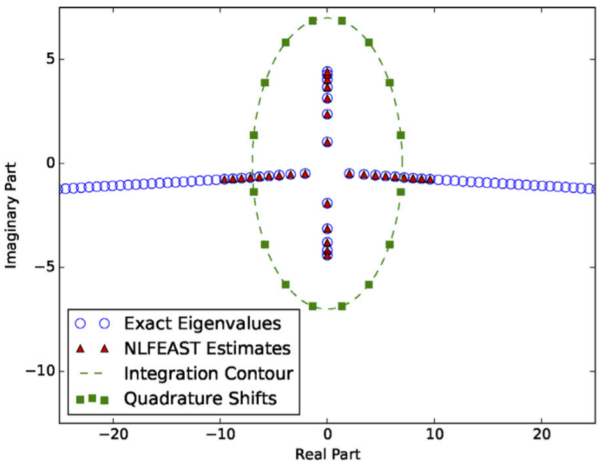

Fig. 3: FEAST algorithm for solving generalized non-linear eigenvalue systems $\mathbf{T}(\lambda)\mathbf{x} = 0$ of size n. We note that at the first iteration where $\mathbf{R}$ is not known, $\mathbf{Y}_j$ can directly be obtained by solving the linear system $\mathbf{T}(z_j)\mathbf{Y}_j = \mathbf{X}$.

Input:
Contour Γ containing m wanted eigenvalues
Set of quadrature nodes and weights $\{z_j, \omega_j\}$
Subspace (random) $\mathbf{X}_{n\times m_0} = \{\mathbf{x}_1, \ldots, \mathbf{x}_{m_0}\}$ with $m_0 \geq m$
While $\{\mathbf{r}_i\}$ not converged for all λ_i inside Γ
Solve $\mathbf{T}(z_j)\mathbf{X}_j = \mathbf{R}$ for all contour nodes j
Compute $\mathbf{Y}_j = (\mathbf{X} - \mathbf{X}_j)(z_j\mathbf{I} - \mathbf{\Lambda})^{-1}$
Compute $\mathbf{Q}_0 = \sum_j \omega_j \mathbf{Y}_j$ and $\mathbf{Q}_1 = \sum_j \omega_j z_j \mathbf{Y}_j$
Perform the QR decomposition $\mathbf{Q_0} = \mathbf{q}_{n\times m_0}\mathbf{r}_{m_0\times m_0}$
Compute $\mathbf{C}_{m_0\times m_0} = \mathbf{q^H Q_1 r^{-1}}$
Solve reduced eigenvalue problem $\mathbf{CW} = \mathbf{W\Lambda}$
Update $\mathbf{X}$=$\mathbf{qW}$, noting that $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_{m_0})$
Form $\mathbf{R} = \{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{m_0}\}$ with $\mathbf{r}_i = \mathbf{T}(\lambda_i)\mathbf{x}_i$
Output: all m eigenpairs $\{\lambda_i, \mathbf{x}_i\}$ inside Γ