Calculating eigenvalues of non-hermitian matrices to determine resonance energies and widths

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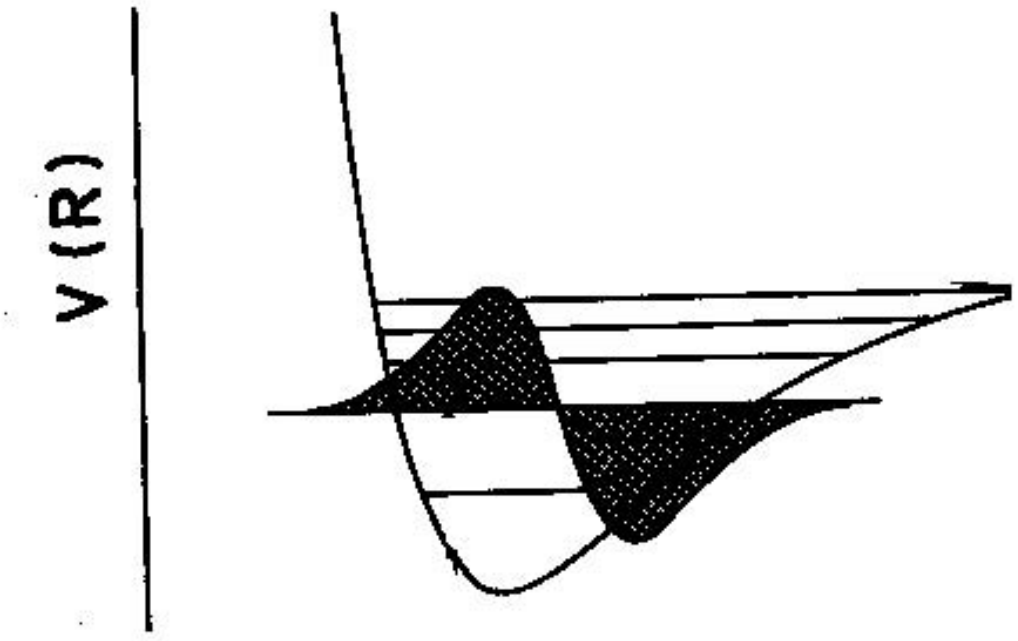
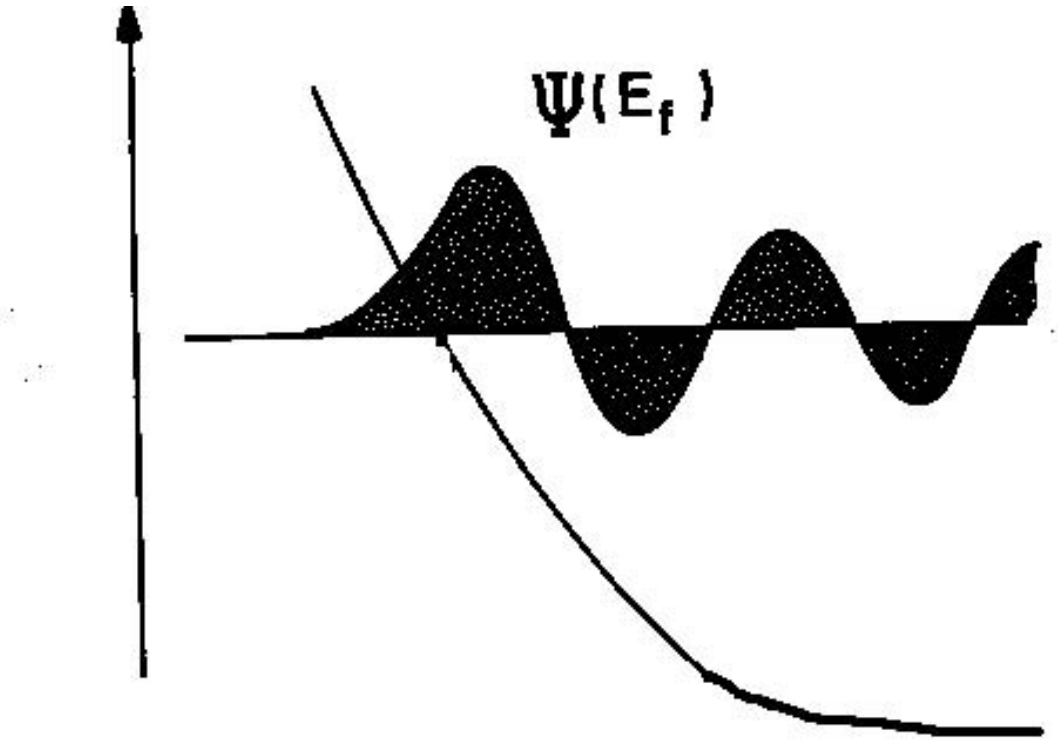
What is a resonance?

Solutions of the Schroedinger equation

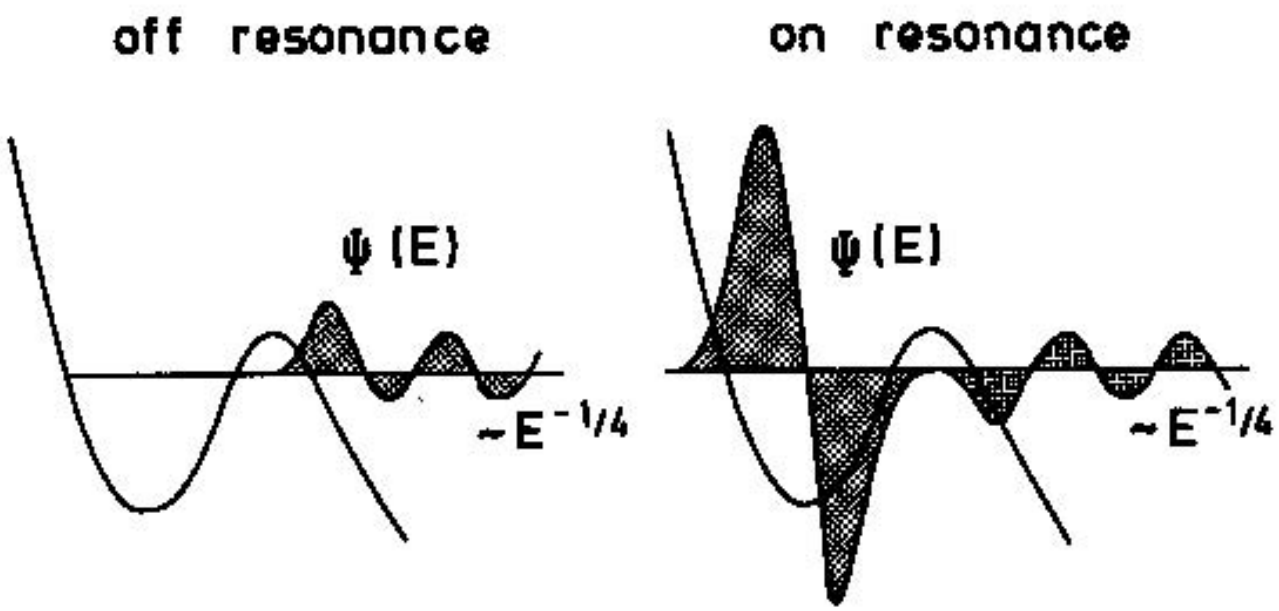
A bound state



A scattering state



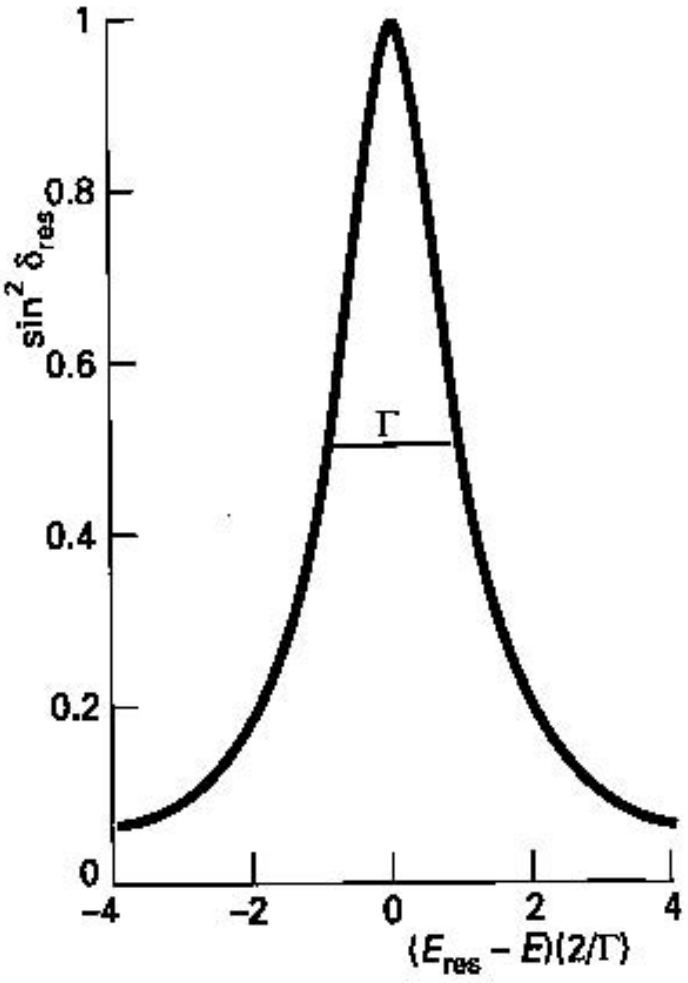
A resonance state



A molecule or complex with a finite lifetime

Resonances are the continuation of the bound states into the continuum

A resonance peak in a spectrum looks like:



It is possible to show that if outgoing boundary conditions are imposed

i.e.

$$\psi \sim e^{+ikr}$$

$$k = \sqrt{2mE}$$

there are solutions of the Schroedinger equation with complex energies

$$E = E_r - i\frac{\Gamma}{2}$$

energy at which resonance occurs width of the resonance

with $\Gamma > 0$

Our goal is to find these states

Problem: ψ diverges

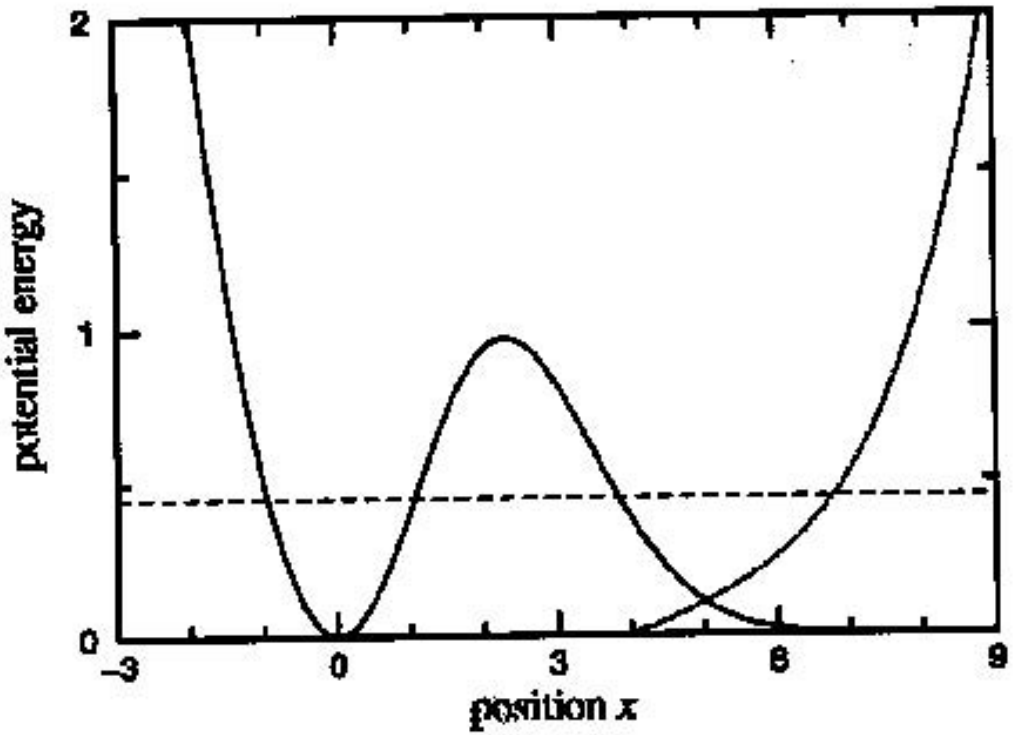
$$E = E_r - i\frac{\Gamma}{2}$$

$$k = k_r - ik_i \quad ; \qquad k_i > 0$$

$$e^{+ikr} \rightarrow e^{+irk_r} e^{+rk_i}$$

Standard Approach

$H \to H - i\eta W \qquad \eta > 0.$



W kills of the divergence

Choose W so that it does not perturb ψ in the interaction region

η is a parameter that is varied to minimise the perturbation

We discretize to obtain a matrix eigenvalue problem

$$(\mathbf{H} - \mathbf{i}\eta\mathbf{W})\mathbf{Y} = \mathbf{Y}\mathbf{E}$$

How do we compute the (complex) eigenvalues?

Complex symmetric Lanczos with no re-orthogonalization

Cullum and Willoughby

This works quite well

Deficiencies of usual implementation

- Complex matrix-vector products

- No eigenvectors $\longrightarrow$ no wavefunctions

New approach

$$(\mathbf{H} - \mathbf{i}\eta\mathbf{W})\mathbf{x_k} = \mathbf{E_k}\mathbf{x_k}$$

$$-i\eta\mathbf{W} = \frac{\mathbf{u_k}}{\mathbf{2}}(\mathbf{I} - \mathbf{D_1}) + \frac{\mathbf{1}}{\mathbf{2u_k}}(\mathbf{I} - \mathbf{D_2})$$

where u_k is defined by $E_k = \left(\frac{u_k}{2} + \frac{1}{2u_k}\right)$

Neumaier and Mandelshtam,
Phy. Rev. Lett. 86 5031 (2001)

$\mathbf{H}$ is scaled so that its eigenvalues are between -1 and +1

$\Downarrow$

Quadratic eigenvalue problem

$$(u_k^2\mathbf{D_1} - 2\mathbf{H}u_k + \mathbf{D_2})\mathbf{x}_k = 0 \ .$$

$$\Downarrow$$

Linearize

$$\mathbf{U}\hat{\mathbf{x}}_k = u_k\hat{\mathbf{x}}_k$$

where $\hat{\mathbf{x}}_k = \begin{pmatrix}\mathbf{x_k}\\ \mathbf{y_k}\end{pmatrix}$

Advantages of U

- $\mathbf{U}$ = real
- cost of a matrix-vector product with $\mathbf{U} \sim$ cost of a matrix-vector product with $\mathbf{H}$
- Ideal for Lanczos because desired eigenvalues are extremal

"Symmetric Indefinite Lanczos Method"

Bai, Ericsson, Kowalski,
Templates for the Solution of Algebraic Eigenvalue Problems

$$\mathbf{U}\hat{\mathbf{x}}_k = u_k\hat{\mathbf{x}}_k \rightarrow \mathbf{UX} = \mathbf{Xu}$$

$$\mathbf{DUX} = \mathbf{DXu}$$

where

$$\mathbf{D} = \begin{pmatrix} \mathbf{D_2} & \mathbf{0} \\ \mathbf{0} & -\mathbf{D_1} \end{pmatrix}$$ is symmetric

Also

$$(\mathbf{DU})^{\mathbf{T}} = \mathbf{U}^{\mathbf{T}}\mathbf{D}^{\mathbf{T}} = \mathbf{U}^{\mathbf{T}}\mathbf{D} = \mathbf{DU}$$

so $(\mathbf{DU})$ is symmetric

But BOTH $(\mathbf{DU})$ and $\mathbf{D}$ are not positive definite

The key idea is to use a $\mathbf{D}$ inner product

Basis vectors are orthogonal wrt an indefinite inner product

- loss of linear independence
- failure of the method

It works best for small matrices and for isolated eigenvalues (shift and invert)

For my purpose it fails

Go back to attempting to solve

$$\mathbf{U}\hat{\mathbf{x}}_k = u_k\hat{\mathbf{x}}_k \rightarrow \mathbf{UX} = \mathbf{Xu}$$

Non-hermitian Lanczos

Two sets of bi-orthogonal vectors formed from the Krylov spaces

$$[\mathbf{q}, \mathbf{Uq}, \mathbf{U^2q}, \cdots] \qquad [\mathbf{p}, \mathbf{U^T p}, (\mathbf{U^T})^\mathbf{2}\mathbf{p}, \cdots]$$

The columns of $\mathbf{V}$ and $\mathbf{W}$ are Lanczos vectors

They are generated with three-term recurrence relations

The coefficients are chosen according to the recipe of Freund and Nachtigal

There are different ways to choose the coefficients consistent with the requirement $\mathbf{v_{i+1}^T w_{i+1} = 1}$

In matrix form the recurrence relations are

$$\mathbf{U V_M = V_{M+1} T_{M+1}}$$

$$\mathbf{U^T W_M = W_{M+1} (\Gamma^{-1} T_{M+1} \Gamma)}$$

$\mathbf{\Gamma}$ = diagonal matrix related to the way the vectors are normalized

eigenvalues of $\mathbf{T_M}$ $\rightarrow$eigenvalues of $\mathbf{U}$

To increase stability and avoid the need to balance we compute eigenvalues of $\mathbf{G^{-1} T_M G}$, where $\mathbf{G}$ = diagonal and $\mathbf{G^{-1} T_M G}$ is symmetric

Chemist's dream

No reorthogonalization

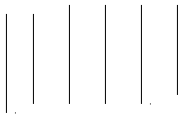
Copied eigenvalues are accurate

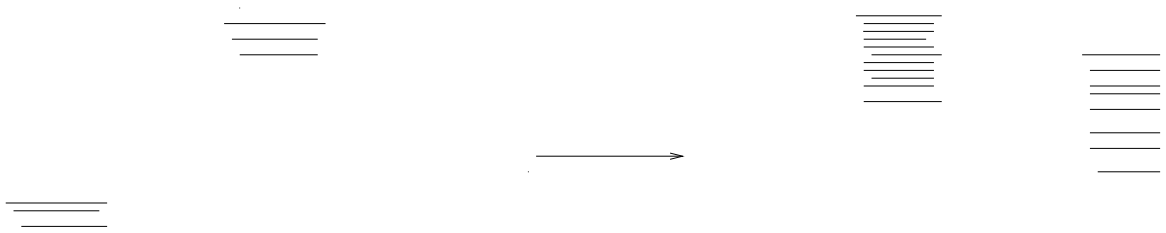
This does not work

Near copies are produced but

$norm$ [*copied e'val of largest norm - copied e'val of smallest norm*]

increases as we increase the number of matrix-vector products





What is the best estimate of the eigenvalue?

If we use the coupled-two-term approach the situation is somewhat better

Generate $\mathbf{p}$ vectors with $\mathbf{v}$ vectors

Generate $\mathbf{q}$ vectors with $\mathbf{w}$ vectors

The four recursion relations for the four sets of factors each involve only 2 vectors

It is not necessary to do matrix-vector products with both $\mathbf{U}$ and $\mathbf{U^T}$

Because $\mathbf{U^T D = DU}$

$$\tilde{\mathbf{w}}_{k+1} = \theta_k \mathbf{D} \tilde{\mathbf{v}}_{\mathbf{k+1}}$$

$$\mathbf{q}_k = \theta_k \mathbf{D} \mathbf{p}_{\mathbf{k}}$$

$\theta_k =$ constant related to the norms of the vectors

Coupled-two-term is better but not good enough (copies are not nearly perfect)

How to compute accurate eigenvalues

- For e'values with norms close to one we identify groups of eigenvalues with almost identical norms

- Average of eigenvalues in a group is $\tilde{u}$

  $\tilde{u}$ = approximate eigenvalue

- Compute approximate right eigenvectors of $\mathbf{T_M}$ by inverse iteration using LU decomposition of $(\tilde{u}\mathbf{I} - \mathbf{T_M}) \rightarrow \mathbf{R}$

- $\mathbf{X_{Lan}^{R} = V_{ID} R}$, where ID = optimal iteration depth (between the number of iterations at which first copy occurs and number at which second copy occurs)

- $\mathbf{X_{Lan}^{L} = D X_{Lan}^{R}}$

-

$$\mathbf{UX = Xu}$$

$$\mathbf{U X_{Lan}^{R} Z = X_{Lan}^{R} Z u}$$

$$\mathbf{[(X_{Lan}^{L})^{T} U X_{Lan}^{R}] Z = [(X_{Lan}^{L})^{T} X_{Lan}^{R}] Z u}$$

$\mathbf{[(X_{Lan}^{L})^{T} X_{Lan}^{R}]}$ is nearly diagonal

- Eigenvalues are computed in groups because to compute them all at once would require storing large $\mathbf{X}_{\mathbf{Lan}}^{\mathbf{R}}$ matrices

Key idea: We use non-hermitian Lanczos ideas to determine a very good subspace and tben extract eigenvalues from it

Disadvantage

- We must store Lanczos vectors on disk

Advantage

- No troubles with instability and inaccuracy

- no complex arithmetic

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