

Modified stochastic variational approach to non-Hermitian quantum systems

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Abstract. The stochastic variational method has proven to be a very efficient and accurate tool to calculate especially bound states of quantum-mechanical few-body systems. It relies on the Rayleigh-Ritz variational principle for minimizing real eigenenergies of Hermitian Hamiltonians. From molecular to atomic, nuclear, and particle physics there is actually a great demand of describing also resonant states to a high degree of reliance. This is especially true with regard to hadron resonances, which have to be treated in a relativistic framework. So far standard methods of dealing with quantum chromodynamics have not yet succeeded in describing hadron resonances in a realistic manner. Resonant states can be handled by non-Hermitian quantum Hamiltonians. These states correspond to poles in the lower half of the unphysical sheet of the complex energy plane and are therefore intimately connected with complex eigenvalues. Consequently the Rayleigh-Ritz variational principle cannot be employed in the usual manner. We have studied alternative selection principles for the choice of test functions to treat resonances along the stochastic variational method. We have found that a stationarity principle for the complex energy eigenvalues provides a viable method for selecting test functions for resonant states in a constructive manner. We discuss several variants thereof and exemplify their practical efficiencies.

1. Introduction

Usually the theory of quantum systems is formulated in a Hilbert space and is based on Hermitian operators for observables [1]. Most calculational methods for solving quantum-mechanical problems are adapted to such a framework. This is particularly true for variational techniques treating bound states. They are based on the fundamental Rayleigh-Ritz theorem for minimizing the energy expectation values by exploiting an ever larger subspace of the full Hilbert space. In particular, the stochastic variational method (SVM), as it is elaborated and outlined, for instance, in [2], is very flexible and well-suited for a wide range of quantum systems, especially because it allows to handle non-linear variational parameters occurring in a given problem (see also [3]).

Resonant quantum systems (with a finite number of exit/decay channels) elude such a conventional treatment. However, they occur in a wide range of different scales from molecules and atoms to nuclear and particle physics. Quantum-mechanical resonances fall outside the discrete and continuous (real) spectra of Hermitian Hamiltonians. They correspond to complex eigenvalues, with the real parts representing the *resonance energies* and the imaginary parts the *decay widths*. The resonance wave functions are not a-priori square-integrable, what makes them inapplicable for directly calculating observables.



As a consequence, conventional variational techniques as characterized above cannot be applied, as they are adapted to eigenfunctions in square-integrable Hilbert spaces $L^2(\mathbb{R}^n)$. A common way out is to apply suitable similarity transformations (e.g., complex scaling), what changes the problem of locating the original resonance positions into finding eigenvalues of a transformed operator on a Hilbert space. This operator is, however, non-Hermitian. Basic strategies for dealing with non-Hermitian quantum-mechanical operators (Hamiltonians) are discussed in [4].

Unfortunately, after such (similarity) transformations are performed, standard variational methods are not directly applicable, since a minimization principle of eigenenergies, such as the Rayleigh-Ritz principle, is not adequate for complex eigenvalues. Rather an alternative selection principle for test functions has to be advocated. Instead of a Rayleigh-Ritz-type minimization a stationarity principle of complex eigenvalues can be designed, which can also deal with non-Hermitian Hamiltonians. Here we show that the SVM can be extended using a generalized selection criterion for test functions based on a stationarity principle. In this way it is made capable of treating also quantum-mechanical resonances in an efficient manner.

The findings presented in this paper are essentially based on results obtained in the master thesis [5], where also the mathematical foundation of the approach is given together with further details and additional examples.

2. Short characterization of resonances

In the conventional setting of quantum mechanics one considers a Hamiltonian

$$\hat{H} = -\frac{1}{2}\Delta + \gamma\hat{V}, \quad (1)$$

given on a square-integrable Hilbert space. It consists of the kinetic energy operator, here suitable normalized corresponding to the Laplacian Δ , and a potential operator $\hat{V}$ with a strength γ . The time evolution is produced by the operator $\hat{U}(t) = e^{-i\hat{H}t}$ (see, e.g., standard text books like [1], [6] or [7]). $\hat{U}(t)$ exists as a unitary operator, if $\hat{H}$ is time-independent and self-adjoint. The quantum-mechanical probability density is preserved and the energy eigenvalues are real. The bound states from the discrete spectrum of a given system (here, for simplicity assumed to be one-dimensional) follow from the eigenvalue equation

$$\hat{H}\psi(x) = E\psi(x) \quad (2)$$

and are represented by poles of the resolvent $\hat{G}(z) = (z - \hat{H})^{-1}$, with $z \in \mathbb{C}^1$, on the negative real axis of the physical sheet of the complex energy plane, whereas the scattering states lie on the branch cut at positive real energies (cf., e.g., [6]).

Resonances of the system, which can, for instance, be transmuted from bound states by reducing the potential strength γ , correspond to poles of the resolvent on the lower half-plane of the unphysical energy sheet and can be observed by sudden changes in the energy dependence of the (ℓ -th partial wave) scattering cross section. This resonance behaviour is usually parametrized by the Breit-Wigner formula

$$\sigma_\ell(E) = \frac{\left(\frac{\Gamma}{2}\right)^2}{(E - E_r)^2 + \left(\frac{\Gamma}{2}\right)^2}, \quad (3)$$

where the pole position is given by $\mathcal{E} = E_r - i\frac{\Gamma}{2}$, with E_r the so-called resonance energy and Γ the resonance decay width.

The poles of the resolvent or equivalently the scattering operator $S_\ell(z)$ are related to zeros of the Jost function $\mathcal{N}_\ell$, which represent the coefficients of the asymptotic parts of the regular

solution $\phi_{\ell k}$ of the Schrödinger equation (2) for $r \rightarrow \infty$

$$\phi_{\ell k}(r) \rightarrow \frac{i}{2} \left[\mathcal{A}(k) \hat{h}_{\ell}^{-}(kr) - \mathcal{A}^{*}(k) \hat{h}_{\ell}^{+}(kr) \right], \quad (4)$$

where $\hat{h}^{\pm}$ are the Riccati-Hankel functions. If we require outgoing boundary conditions and $\mathcal{A}(k)=0$ for a certain complex momentum k , i.e. a resonance pole at $k = k_r - ik_i$, where $k_r, k_i \in \mathbb{R}^1$ and $k_i > 0$, we get

$$\phi_{\ell k}(r) \rightarrow C e^{ikr} = C e^{ik_r r} \cdot e^{k_i r} \rightarrow \infty \quad (5)$$

as $r \rightarrow \infty$. This means $\phi_{\ell k} \notin L^2(\mathbb{R}^n)$ and therefore unsuitable for the calculation of observables.

3. Non-Hermitian Hamiltonians and c-product

3.1. Complex Hamiltonians

Asymptotically rising resonance wave functions (residues at complex poles, sometimes also termed Gamow functions) $\psi(x)$ can be regularized by similarity transformations (see [4]):

$$\psi_S = \hat{S}\psi, \quad \hat{H}_S = \hat{S}\hat{H}\hat{S}^{-1}. \quad (6)$$

The most important property of such transformations is that the eigenvalue spectrum of the original Hamiltonian remains invariant with the respective eigenstates:

$$\hat{H}\psi = \lambda\psi, \quad \hat{H}_S\psi_S = \lambda\psi_S, \quad \lambda \in \mathbb{C}^1. \quad (7)$$

Most frequently used is the complex-scaling method, which consists in rotating the space variable by a certain angle θ

$$(\hat{S}_{\theta}\psi)(x) = \psi_{\theta}(x) = \tilde{\psi}(e^{i\theta}x), \quad (8)$$

where $\tilde{\psi}$ is understood as the analytic continuation of ψ onto a suitable domain of rotated coordinates. This transformation makes ψ_{θ} asymptotically well-behaved for a desired range of momenta k

$$(\hat{S}_{\theta}\psi)(x \rightarrow \infty) \sim \exp(i e^{i\theta} k x) = e^{ik'x}, \quad (9)$$

where $k' = e^{i\theta}k$ and thus $\text{Im } k' > 0$. Evidently, the complex-scaling transformation turns the Hamiltonian complex

$$\hat{H}_{\theta} = -\frac{1}{2}e^{-2i\theta}\Delta + \gamma\hat{V}(e^{i\theta}x), \quad (10)$$

where, of course, analyticity of the potential $\hat{V}$ is required in the required domain.

Complex Hamiltonians may arise in a number of further cases related to resonances. For instance, a coupled-channels theory involving resonance decay channels produces a complex optical potential after a Feshbach reduction (see, e.g., [8]). For energies above the resonance threshold the corresponding reduced Hamiltonian will thus acquire an imaginary part and lead to complex eigenvalues relating to a resonance at $\mathcal{E} = E_r - i\frac{\Gamma}{2}$.

Standard variational methods adhering to the Rayleigh-Ritz principle cannot be applied to solving the eigenvalue problem of a complex Hamiltonian like in Eq. (10) or similar. A possible way out is a stationarity principle for finding the right position of the resonance poles. A prerequisite for formulating such a stationarity principle is the definition of an alternative to the usual scalar product on a Hilbert space.

3.2. *c-product*

The introduction of the *c-product* $(\cdot|\cdot)$ provides a substitution for the common scalar product $\langle\cdot|\cdot\rangle$ in case of non-Hermitian Hamiltonians. It is defined through the mapping $L^2(\mathbb{R}^n) \times L^2(\mathbb{R}^n) \rightarrow \mathbb{C}^1$ by

$$(\phi|\psi) = \int_{\mathbb{R}^n} \phi(x)\psi(x) dx. \quad (11)$$

With the *c-product* many of the usual properties of the inner product are carried over to the non-Hermitian case. Suppose that ϕ_S and ψ_S are similarity-transformed eigenstates of $\hat{H}_S$, then in particular

- $|(\phi|\psi)| \leq \|\phi\| \|\psi\|$, $\forall \phi_S, \psi_S \in L^2(\mathbb{R}^n)$, i.e. the Cauchy-Schwartz inequality holds, and
- $(\phi_S|\hat{H}_S\psi_S) = (\hat{H}_S\phi_S|\psi_S) := (\phi_S|\hat{H}_S|\psi_S)$, i.e. $\hat{H}_S$ is "Hermitian" with respect to the *c-product*.

Similarly, the orthogonality property for eigenstates corresponding to different eigenvalues is guaranteed by the *c-product*.

4. Stationarity principle and the SVM

We are now prepared to formulate the stationarity principle for the selection of basis functions in a variational approach to non-Hermitian problems and to apply it especially in the SVM.

4.1. *Stationarity principle*

Given the similarity-transformed eigenvalue problem as in Eq. (7), we consider the Rayleigh quotient

$$R(\phi_S) = \frac{(\phi_S|\hat{H}_S|\phi_S)}{(\phi_S|\phi_S)}. \quad (12)$$

Then for some arbitrarily varied state $\phi_S = \psi_S + \epsilon\delta\psi_S$, with $\epsilon \rightarrow 0$, one gets

$$R(\phi_S) = \lambda + O(\epsilon^2), \quad (13)$$

i.e. ψ_S is a critical point of R , where the critical value is the exact eigenvalue of $\hat{H}_S$.

In the context of a variational calculation searching for the optimal solution of a non-Hermitian eigenvalue problem, we consider $\psi_S(\alpha)$ as a function of a set of (non-linear) parameters $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_r) \in \mathbb{C}^r$. If for a particular set α^0 the eigenvalue equation is satisfied and $(\psi_S(\alpha^0)|\psi_S(\alpha^0)) \neq 0$, then

$$\frac{\partial R(\alpha^0)}{\partial \alpha^i} = 0, \quad \forall \alpha_i. \quad (14)$$

This means that we have to look for a stationary energy eigenvalue in order to find the optimal (non-linear) variational parameters.

The linear variational parameters a_k of an expansion into test functions χ_k

$$\psi_S = \sum_{k=1}^{\infty} a_k \chi_k \approx \sum_{k=1}^N a_k \chi_k \quad (15)$$

can be determined as usual by the solution of the following system of equations:

$$\sum_{l=1}^N (\chi_k|\hat{H}_S|\chi_l) a_l = \lambda \sum_{l=1}^N (\chi_k|\chi_l) a_l. \quad (16)$$

4.2. Modified SVM

The stationarity principle outlined above can directly be applied for the random selection of basis functions in the SVM for non-Hermitian problems. Several variants are still possible. We have checked the performance of different selection criteria for the case of the Rittby potential (see Fig. 1)

$$V(x) = \left(\frac{1}{2}x^2 - J \right) e^{-\beta x^2} \quad (17)$$

with parameters $J = 0.8$ and $\beta = 0.1$, such that exactly one bound state is supported, shown by the (red) level on the l.h.s. of Fig. 1. The exact solutions for its resonances are known from the literature [9] or can be generated by alternative methods, such as the finite-difference discretisation after complex scaling as in [5].

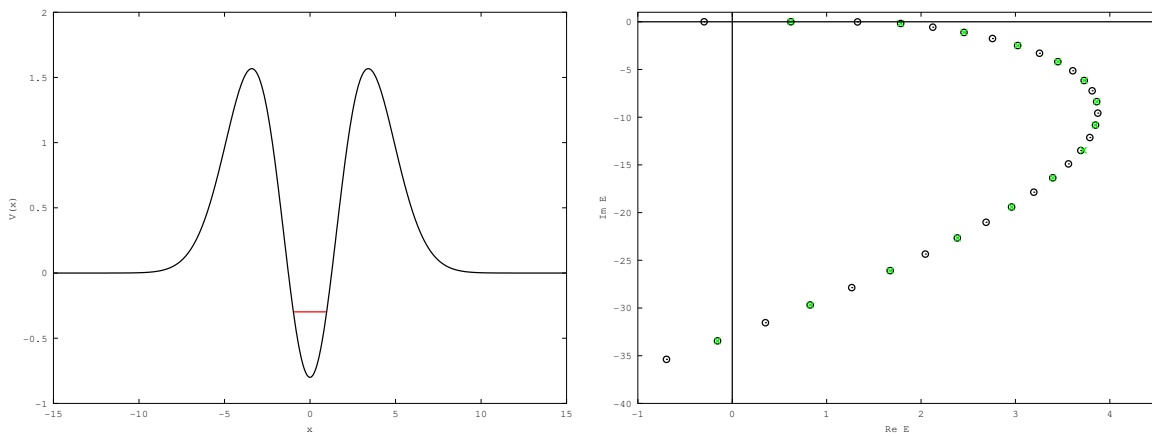


Figure 1. Spatial dependence of the Rittby potential (left) and its eigenvalues, as calculated with the finite-difference method (right). The (green) crosses are the results from [9] available for odd- n eigenvalues.

Application of the stationarity principle to the SVM with random selection of basis functions yields the results shown in Fig. 2. We have also tried additional criteria for the selection of test functions in order to explore speeding up the convergence. Among them were notably (for details see [5])

- the gradient method, i.e. the selection of test functions based on the minimization of the norm of the multi-dimensional gradient in the space of non-linear parameters

$$\nabla R^T = \left(\frac{\partial R}{\partial \alpha_1} \dots \frac{\partial R}{\partial \alpha_r} \right), \text{ and}$$

- a weight-based update strategy together with the orthonormalisation of the basis (ONB), where the least-relevant test functions are always omitted before generating new ones.

The rates of convergence for the three selection criteria described above are shown in Fig. 3. Again we exemplify them for the particular case of the $n=3$ resonance of the Rittby potential, whose exact position is at $\mathcal{E}_3 = 1.7846 - i0.1738$. As a measure we use the absolute values $|\mathcal{E}_3 - \mathcal{E}_3^{\text{approx}}|$, where $\mathcal{E}_3, \mathcal{E}_3^{\text{approx}} \in \mathbb{C}^1$, the latter being the approximate eigenvalue in each step.

It appears that improvements over a pure random selection of basis functions can be achieved by the more refined selection criteria outlined above. Especially the weight-based method with ONB immediately improves the approximation already with moderate basis sizes. The best accuracy of about 10^{-7} , which is probably sufficient for most applications, is reached for $N \approx 70$ test functions. For even bigger bases this precision is lost again, presumably due to the fact

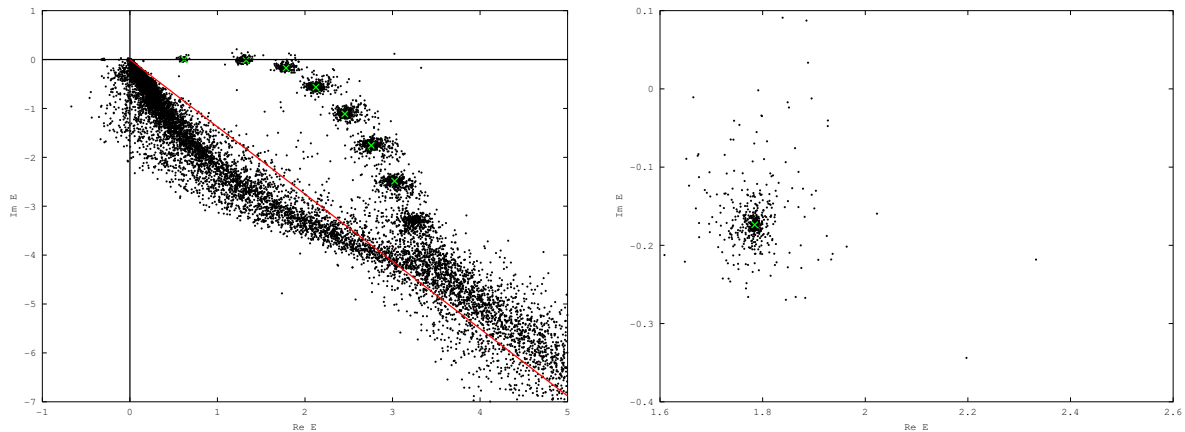


Figure 2. Left: Approximate eigenvalues (black dots) from stochastically selecting $N = 40$ random basis functions and varying only the linear parameters, according to the stationarity principle for the Rittby potential (17); 500 runs are combined. The (green) crosses give the exact resonance positions. Right: Zoomed distribution around the $n=3$ resonance.

that in this case the eigenvalue problem becomes badly conditioned. The gradient method offers itself as a straightforward and efficient tool for generating a reliable basis. It outperforms the random stochastic selection starting from a basis size of $N \approx 40$ and reaches its highest accuracy of $\leq 10^{-7}$ beyond $N \approx 80$.

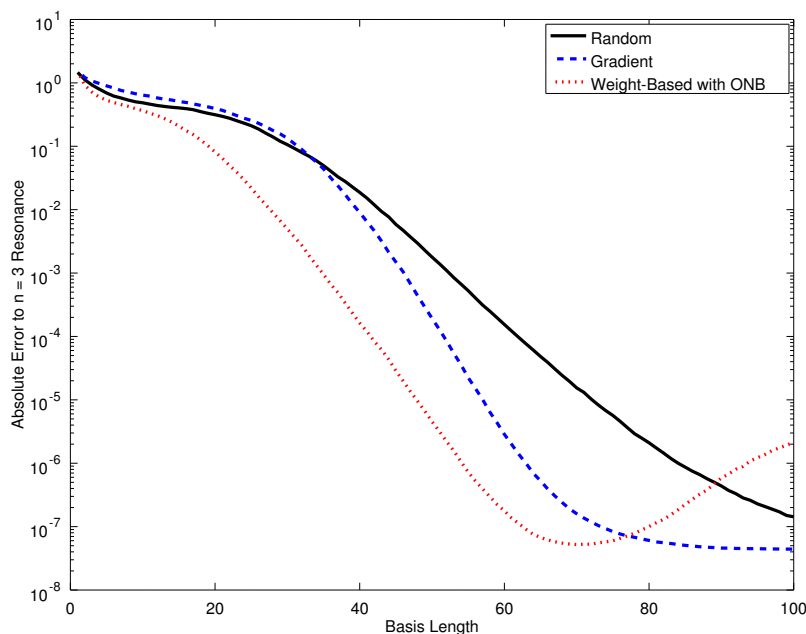


Figure 3. Convergence of the absolute error in the resonance position in case of the $n=3$ resonance of the Rittby potential (17) for different selection criteria of the basis (see the text): Random (solid/black), gradient (dashed/blue) and weight-based with orthonormalisation of the basis (dotted/red).

5. Conclusions

In this paper our main goal has been especially the adaptation of the SVM for the treatment of quantum-mechanical resonances associated with complex eigenvalues (i.e. poles in the lower half-plane of the unphysical sheet of the complex energy plane). They are governed by non-Hermitian Hamiltonians, which arise, for instance, from the use of complex optical potentials or after similarity transformations, such as the Zel'dovich or complex-scaling transformations. Since the Rayleigh-Ritz variational principle is not applicable in such cases, we advocated a stationarity principle for the energy expectation value. It has proven suitable for optimizing the linear and non-linear variational parameters within the SVM approach.

Along with the generalisation of the variational principle, we also studied refined criteria for selecting good candidate basis functions in the SVM. In addition to a purely stochastic selection of basis functions in the search for the non-linear variational parameters, we examined a gradient-based search as well as a weight-based method, replacing basis functions with small expansion coefficients by more relevant ones. Thereby we arrived at two particular variants of the SVM that can be applied to non-Hermitian problems in an efficient manner. They turned out to perform significantly better than a purely random basis selection or even a straight-forward finite-difference discretisation of the Hamiltonian.

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