Complex conjugate pairs in stationary Sturmian eigenstates

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Sturmian eigenstates specified by stationary scattering boundary conditions are particularly useful in contexts such as forming simple separable two nucleon t matrices, and are determined via solution of generalized eigenvalue equation using real and symmetric matrices. In general, the spectrum of such an equation may contain complex eigenvalues. But to each complex eigenvalue there is a corresponding conjugate partner. In studies using realistic nucleon-nucleon potentials, and in certain positive energy intervals, these complex conjugated pairs indeed appear in the Sturmian spectrum. However, as we demonstrate herein, it is possible to recombine the complex conjugate pairs and corresponding states into a new, sign-definite pair of real quantities with which to effect separable expansions of the (real) nucleon-nucleon reactance matrices.

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Sturmian states are solutions of Schrödinger-like equations in which the energy is treated as a continuous parameter and the strength of the potential plays the role of the spectral variable [1]. Although at positive energies often one solves [2] the Sturmian equations with outgoing boundary conditions (thereby obtaining eigenvalues and states which are complex), it is convenient sometimes to evaluate the Sturmian eigenstates under stationary boundary conditions [3]. Those states are particularly useful in forming separable expansions of the nucleon-nucleon (NN) reactance (K) matrices, and the process of so doing defines the Sturmian splitting method (SSM) [4]. Therein, the stationary Sturmian expansion was used to separate those K matrices into two groups. Each group is a sign-definite separable representation in itself, one set having attractive and the other having repulsive character. In fact, a set of separable K matrices was generated and the Heitler equation used to specify the t matrices thereafter. The process however allows us to avoid any pathology in the related t matrices due to vanishing on-shell phase shifts (or the equivalent coupled channel relation). Such pathologies do occur [5,6] when other similar separable expansion methods [7] are used with realistic (NN) interactions.

To evaluate stationary Sturmian eigenstates, we solve a generalized eigenvalue equation with purely real, symmetric matrices. Naively one might believe that the corresponding (stationary) eigenvalues and states would also be real. But that is not necessarily the case. If the potential term in the eigenvalue equation has both an attractive and repulsive character, as with realistic NN interactions, degeneracies in the eigenvalues lead to some of them becoming complex. However, those eigenvalues always occur in complex conjugate pairs (CCP's) and, with a simple recombination of such eigenvalues and states, equivalent pairs can be defined that are purely real and have opposite signs. With them, all contributions to the resultant sum in the K-matrix expansion are real and sign definite.

We give now a basic outline of how the Sturmian eigenvalues are determined, and describe why and where these CCP's occur.

To evaluate Sturmian eigenstates, $[\phi^{(P)}_{l,s}(q;E)]$, under stationary boundary conditions, in momentum space one must solve the generalized eigenvalue problem [8],

$$\sum_l \int_0^\infty U^{(P)}_{Ll}(p,q;E)\phi^{(P)}_{l,s}(q;E)q^2dq = \eta^{(P)}_s(E)\sum_l \int_0^\infty V_{Ll}(p,q)\phi^{(P)}_{l,s}(q;E)q^2dq, \tag{1}$$

where $V_{ll'}(p,q)$ is the momentum space interaction, and $U^{(P)}_{LL'}(p,q;E)$ is given by the principal value of the second-order Born term, i.e.

$$U^{(P)}_{LL'}(p,p';E) = \sum_l \mathbf{P}\int_0^\infty \frac{1}{E-q^2}V_{Ll}(p,q)V_{lL'}(q,p')q^2dq. \tag{2}$$

The superscript (P) denotes use of the stationary boundary conditions. It is convenient to define the Sturmian expansion via

$$\chi_{L,s}(p';E) = \sum_l \int_0^\infty V_{Ll}(p',q)\phi_{l,s}(q;E)q^2dq\ , \tag{3}$$

in terms of which the (real) K matrices are specified by [4]

$$K_{LL'}(p',p;E) = -\sum_{s=1}^{\infty} \chi_{L,s}^{(P)}(p';E) \left\{ \frac{1}{\eta_s^{(P)}(E)(1-\eta_s^{(P)}(E))} \right\} \chi_{L',s}^{(P)}(p;E). \quad (4)$$

As the K matrices are real, one might expect the eigenvalues (η) and states (χ) to be real also. But that is not always the case. Indeed for positive energies, eigenvalues that are CCP's occur whenever the interaction produces degenerate eigenvalues. Further development is needed to ensure that when such occur, the separable expansions of the K matrices remain real.

We consider first a special interaction studied previously [5], and with which the stationary Sturmian eigenstates are analytic. In this case the states $\chi_s(p;E)$ may be written as

$$\chi_s(p;E) = t_{11}^{-1} a_{1,s}(E) u_1(p) + t_{22}^{-1} a_{2,s}(E) u_2(p) \ , \quad (5)$$

where the two components, t_{ii} [5], have differing signs, and the two energy dependent coefficients $a_{i,s}$ are solutions of the real nonsymmetric standard 2×2 eigenvalue problem

$$\sum_{j=1,2} \mathbf{G}_{i,j}^{(P)} t_{jj}^{-1} a_{j,s} = \eta_s^{(P)} a_{i,s} \ . \quad (6)$$

Here $\mathbf{G}_{i,j}^{(P)} = t_{ii}\delta_{ij} - P_{ij}$, where P_{ij} is given by Eq. (3.2) of Ref. [5].

The result is that a complex conjugated pair appears in the spectrum when the on-shell momentum (k) is in the range (0.26–0.29) fm^{-1}. Outside of that range, and, for $E < 0$, the two eigenvalues are real. In this problem, the two eigenvalues are the roots of a binomial equation, and one finds that at the extremities of this interval, the two real eigenvalues are degenerate. From this, one may observe that CCP's result only if the potential has both an attractive and a repulsive character.

We now consider just how the generalized eigenvalue equations can be solved numerically. The integrals in the semi-infinite interval $[0,\infty]$ of Eq. (1) are found [8] using a standard Gauss-Laguerre N-point quadrature formula with which this equation is transformed into a generalized $2N \times 2N$ matrix eigenvalue problem

$$\sum_{j=1}^{2N} \mathbf{U}_{i,j}^{(P)} a_{j,s} = \eta_s^{(P)} \sum_{j=1}^{2N} \mathbf{V}_{i,j} a_{j,s} \ , \quad (7)$$

where

$$a_{j,s} = k_j^2 w_j \phi_{0,s}^{(P)}(k_j,E) \ \text{ if } j \le N,$$
$$a_{j,s} = k_{(j-N)}^2 w_{(j-N)} \phi_{2,s}^{(P)}(k_{(j-N)},E) \ \text{ if } j > N \ , \quad (8)$$

and k_j and w_j are the points and weights of the quadrature formula.

The matrices $\mathbf{U}^{(P)}$ and $\mathbf{V}$ are real and symmetric and so if $\mathbf{V}$ is nonsingular and positive (or negative) definite, the generalized eigenvalues are real and finite. But for realistic NN interactions, the matrix $\mathbf{V}$ is not sign definite and therefore the generalized spectrum of Eq. (7) may then contain CCP's of eigenvalues (and associated eigenvectors), in agreement with the general theorem for generalized eigenvalue problems [9].

The same equation holds for negative energies where stationary Sturmian eigenstates now coincide with Weinberg's states. These eigenvalues are known to be real in spite of the fact that $\mathbf{V}$ is not sign definite since it can be shown that the states $|\chi\rangle$ satisfy an equivalent generalized equation of the type

$$\mathbf{G}(E)\mathbf{V}\mathbf{G}(E) \ |\chi_s\rangle = \eta_s(E)\mathbf{G}(E) \ |\chi_s\rangle \ , \quad (9)$$

and in which, for $E < 0$, no singularity occurs. Both matrices are real and symmetric and for $E < 0$, $\mathbf{G}(E)$ is clearly negative definite. Therefore the eigenvalues are real.

As a second example we considered the positive energy, generalized stationary spectrum for the $^1S_0$ Reid soft core potential [10]. At 100 and 200 MeV all the eigenvalues are real. But at 140 MeV, a CCP appears having the value $(-0.33 \pm i0.02)$ fm^{-1}. It is a quite stable result, changing little in value with variation either of the set of grid points or of the energy (around 140 MeV). That CCP disappears between 189 and 190 MeV being replaced (at 190 MeV) by two real eigenvalues. Those two real eigenvalues are almost degenerate and are comparable with the real part of the 189 MeV CCP. Thus the CCP has not originated from round off errors due to numerical approximations. Rather it is an actual characteristic of the spectrum.

As indicated previously, we seek a technique to eliminate use of these CCP's in, for example, the specification of separable representations of NN operators using the SSM scheme. This is achieved by first grouping those CCP's into an attractive (+) and a repulsive (−) subspace according to the following criteria. Given that we can define the total contribution of a CCP in the K-matrix expansion as

$$K_{LL'}^{\text{ccp}}(p,p';i) = -[\chi_{L,i}^{(P)}(p)\mu_i\chi_{L',i}^{(P)}(p') + \{\chi_{L,i}^{(P)}(p)\mu_i\chi_{L',i}^{(P)}(p')\}^*] \ , \quad (10)$$

where

$$\mu_i \equiv \frac{1}{[\eta_i^{(P)}(1-\eta_i^{(P)})]} \ . \quad (11)$$

We can also define the eigenvalue as

$$\mu_i \equiv \sigma_i + i\tau_i \ , \quad (12)$$

and the eigenstate as

$$\chi_{L,i}^{(P)}(p) \equiv f_{L,i}(p) + ig_{L,i}(p) \ . \quad (13)$$

Now defining a new pair of eigenvalues with opposite sign via

$$\mu_i^{\pm} \equiv \pm \frac{2}{|\eta_i^{(P)}(1-\eta_i^{(P)})|} \ , \quad (14)$$

we obtain two purely real quantities, namely,

$$\mu_i^+ = 2\sqrt{\sigma_i^2+\tau_i^2},$$
$$\mu_i^- = -2\sqrt{\sigma_i^2+\tau_i^2}\ . \tag{15}$$

Similarly, defining the attractive and repulsive eigenstates as

$$\chi_{L,i}^+(p) = a_1^+ f_{L,i}(p) + a_2^+ g_{L,i}(p),$$
$$\chi_{L,i}^-(p) = a_1^- f_{L,i}(p) + a_2^- g_{L,i}(p)\ , \tag{16}$$

the a coefficients are also purely real and are specified by

$$a_1^+ = \frac{1}{\sqrt{2}}\frac{\sqrt{\sqrt{\sigma_i^2+\tau_i^2}+\sigma_i}}{\sqrt[4]{\sigma_i^2+\tau_i^2}},$$
$$a_2^+ = \frac{-\tau_i}{\sqrt{2}|\tau_i|}\frac{\sqrt{\sqrt{\sigma_i^2+\tau_i^2}-\sigma_i}}{\sqrt[4]{\sigma_i^2+\tau_i^2}},$$
$$a_1^- = \frac{1}{\sqrt{2}}\frac{\sqrt{\sqrt{\sigma_i^2+\tau_i^2}-\sigma_i}}{\sqrt[4]{\sigma_i^2+\tau_i^2}},$$
$$a_2^- = \frac{\tau_i}{\sqrt{2}|\tau_i|}\frac{\sqrt{\sqrt{\sigma_i^2+\tau_i^2}+\sigma_i}}{\sqrt[4]{\sigma_i^2+\tau_i^2}}\ . \tag{17}$$

It is possible then to redefine Eq. (10) as

$$K_{L,L'}^{\rm ccp}(p,p';i) = -\{\chi_{L,i}^+(p)\mu_i^+\chi_{L',i}^+(p') + \chi_{L,i}^-(p)\mu_i^-\chi_{L',i}^-(p')\}\ , \tag{18}$$

where the term $K_{L,L'}^{\rm ccp}(p,p';i)$ splits into two contributions in which each element of the CCP contributes an equal amount to the attractive and the repulsive quantities.

In summary, we have shown that CCP's may appear in the stationary Sturmian spectrum for certain energy range. When this is the case, the Sturmian eigenstates become degenerate at the edge of these intervals leading to the transition from a real to a complex eigenspectrum. The occurrence of such CCP's and corresponding eigenstates leads to terms in the Sturmian expansion which are neither real nor sign definite; a coincidence which does not allow straightforward application of the SSM. However, a proper recombination of the two complex conjugate states leads to new ones which are real and sign definite and with which application of the SSM in the presence of CCP's can be made.

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