Bipartite correlations in quantum resonance states

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We discuss a diagonal representation of a reduced density matrix determined within the framework of the complex scaling method. We also discuss a possible measure of bipartite correlations in quantum resonance states. As an example, we consider a one-dimensional system of two bosons with a contact interaction subjected to an open potential well. The correlation properties of the lowest-energy resonance state of the system are explored over a wide range of the inter-boson interaction strength, including the Tonks-Girardeau regime.

I. INTRODUCTION

Quantum entanglement is a fundamental feature of the quantum world and has attracted significant research attention. New experimental techniques have opened up opportunities for practical applications of quantum entanglement in various branches of information technology [1, 2]. The fields of quantum teleportation, quantum cryptography and quantum computation have grown particularly rapidly in the last few years. Entanglement is also used as an alternative measure of correlation in systems of interacting particles [3]. Considerable efforts have been made to understand quantum correlations in bound states of model systems such as the Moshinsky atom [4, 5], quantum dot systems [6, 13] or ultra-cold boson systems [14–18]. Moreover, in recent years, the helium atom and helium-like ions have been extensively studied in this context [19–29]. For an overview of the recent developments in studies of entanglement in quantum composite systems, see [30].

However, relatively few attempts have been made to improve understanding of the correlation properties of systems that exhibit metastable states. Various theoretical methods to determine resonance energies and lifetimes can be found in the literature. Among these, the most popular are the complex scaling method (CSM) [31] and the real stabilization method [32]. Treatment of the entanglement of resonance states with the CSM was proposed in [9], where both a complex-scaled density operator and a complex linear entropy were introduced. Within the framework of this formalism, the resonance states of two-electron Gaussian quantum dots have recently been analyzed from the perspective of quantum information [33]. Nonetheless, as far as we know, no study has discussed in detail the diagonal representation of the complex-scaled reduced density matrix. This gap in the literature provides the motivation for the present Letter.

The remainder of this Letter is structured as follows. Section II briefly outlines the CSM. Section III discusses the diagonal form of the reduced density matrix determined in the framework of the CSM. Section IV discusses possible correlation measures for resonance states. Section V focuses on the correlation properties of systems that contain two interacting bosons trapped inside an open potential well. Finally, Section VI presents concluding remarks.

II. THE COMPLEX SCALING METHOD

The CSM is a powerful tool for searching for the resonant parameters of a system that supports metastable states [31]. The utility of this method is that the resonant states can be treated by applying the methods used to compute bound states, for example, a finite-basis-set approximation [34, 35]. Here we only briefly outline the complex scaling formalism. Details of the computational technique of the CSM can be found in an excellent overview [31].

In the CSM, the Hamiltonian \( \tilde{H} = \tilde{T}(x) + \tilde{V}(x) \), where \( \tilde{T} \) and \( \tilde{V} \) are kinetic and potential energy operators, respectively, is transformed by coordinate transformation \( x \to xe^{\theta i} \) into

\[
\tilde{H}^\theta = e^{-2\theta i}\tilde{T}(x) + \tilde{V}(xe^{\theta i}),
\]

where \( \theta \) is the so-called scaling angle. A key aspect of the CSM is that the complex-scaled Hamiltonian \( \tilde{H}^\theta \) is a non-Hermitian operator and the inner product is defined as

\[
\langle \psi | \varphi \rangle = \int_{\text{all space}} \psi^*(x) \varphi(x) dx,
\]

\[
\langle \varphi | \psi \rangle = \varphi_0(x) \text{ and } \langle \varphi | \psi \rangle = \psi_0(x). \]

The right (\( R \)) and left (\( L \)) eigenstates of \( \tilde{H}^\theta \) are defined by \( \tilde{H}^\theta |\psi_k^R\rangle = W_k^R |\psi_k^R\rangle \) and \( \langle \psi_k^R | \tilde{H}^\theta = \langle \psi_k^L | W_k^L \rangle \), respectively. These equations can be turned into algebraic problems by expanding \( |\psi_k^R\rangle \) and \( |\psi_k^L\rangle \) as linear combinations of \( |\varphi_j\rangle \) and \( |\varphi_k^\dagger\rangle \), respectively, where \{\( |\varphi_j\rangle \)\} is a complete set of orthonormal functions, \( \langle \varphi_i^\dagger | \varphi_j \rangle = \delta_{ij} \). Thus, the first equation becomes the eigenvalue problem \( (H - iW) \delta_l = \delta_l \) with \( H = \langle \varphi_k^\dagger | \tilde{H}^\theta | \varphi_k \rangle \), the eigenvalues of which \( W_{\text{diag}} = \text{diag}(W_0, W_1, \ldots) \) (if \( H \) is diagonalizable) are given by \( W_{\text{diag}} = R^{-1} HR \), where \( R \) is the eigenvector matrix of \( H \). The second equation becomes the eigenvalue problem \( (H^T - iW^T) \hat{L} = \hat{0} \). Because \( W_{\text{diag}} = W_{\text{diag}}^T = (R^{-1} HR)^T = (HR)^T (R^{-1})^T = R^T H^T (R^{-1})^T \), it immediately follows that the eigenvector matrix of the matrix \( H^T \) is \( L = (R^{-1})^T \) and...
Because $R^{-1}R = I$, the family $\{\psi^L_i, \psi^R_i\}$ forms a complete set of orthonormal functions with respect to the inner product (2), that is, $\langle \psi^L_i | \psi^R_j \rangle = \delta_{ij}$. In particular, if $\{\varphi_i\}$ is a real basis and $H$ is a symmetric matrix ($H = H^T$), that is, $W_{\text{diag}} = W^T_{\text{diag}} = (R^T HR)^T = R^T H^T R$ ($R^{-1} = R^T$), then the right and left wavefunctions can alternatively be expressed in the same form, namely $\psi^L_i(x) = \sum_k (R)_{ki} \varphi_k(x)$, where $R^T R = I$. However, in the case of $H^T = H^\ast$ ($H$ is Hermitian), that is, $W_{\text{diag}} = W^\ast_{\text{diag}} = (R^\ast HR)^\ast = R^T H^\ast R^\ast = R^T$, they can be written as $\psi^L_i(x) = \sum_k (k)_{ji} \varphi_k(x)$ and $\psi^R_i(x) = \sum_k (R^\ast)_{ki} \varphi^\ast_k(x)$, where $R^T R = I$. Note that our conclusions coincide with those of (31).

The resonances appear as $\theta$-independent complex eigenvalues $W_k$ with $\text{Im}[W_k] < 0$ (32), and the resonance energies $E_k^{\text{rez}}$ and lifetimes $\Gamma_k$ are obtained as $E_k^{\text{rez}} = \text{Re}[W_k]$ and $\Gamma_k = -2\text{Im}[W_k]$, respectively:

$$W_k = E_k^{\text{rez}} - i \frac{\Gamma_k}{2}. \quad (5)$$

**III. COMPLEX-SCALED REDUCED DENSITY MATRICES**

Suppose we divide a system into two parts, $A$ and $B$. Let us express the right and left wavefunctions of a given resonance state as follows:

$$|\psi^R \rangle = \sum_{ij} c^R_{ij} |a_i \rangle_A \big|b_j \rangle_B, \quad (6)$$

and

$$\langle \psi^L | \langle = \sum_{kl} c^L_{kl} A \langle a_k | B \langle b_l |. \quad (7)$$

Here, $\langle \psi^L | \psi^R \rangle = 1$, where $\{a_i\}$ and $\{b_j\}$ are bases of square integrable orthonormal functions for the subsystems $A$ and $B$, respectively, $A \langle a_i | a_j \rangle_A = \delta_{ij}$, $B \langle b_i | b_j \rangle_B = \delta_{ij}$. Following (2), we define the density operator as

$$\hat{\rho}^{AB} = |\psi^R \rangle \langle \psi^L|. \quad (8)$$

The reduced density matrix of subsystem $A$ is thus obtained by tracing out the $B$ degrees of freedom, which gives

$$\hat{\rho}_A = \text{tr}_B[\hat{\rho}^{AB}] = \sum_{ik} \rho^A_{ik} |a_i \rangle_A \langle a_k |. \quad (9)$$

where $\rho^A_{ik} = \sum_j e^R_{ij} e^L_{kj}$. Its right and left eigenstates are defined by $\hat{\rho}_A |u^R_n \rangle_A = \lambda_n |u^R_n \rangle_A$ and $A \langle u^L_n | \hat{\rho}_A = A \langle u^L_n | \lambda_n$, respectively. In strict analogy with Section III we conclude that

$$|u^R_n \rangle_A = \sum_j (V)_{jn} |a_j \rangle_A, \quad (10)$$

and

$$A \langle u^L_n | = \sum_j (V^{-1})^T_{jn} A \langle a_j |, \quad (11)$$

where $V$ is the eigenvector matrix of the matrix $\rho_A = [A \langle a_i | \hat{\rho}_A | a_k \rangle_A] = [\rho^A_{ik}]$ with the eigenvalues $\lambda^A_n (\lambda_n = \lambda^A_n)$. $A \langle u^L_n | u^R_m \rangle_A = \delta_{nm}$. Following on from the above, $\hat{\rho}_A$ can be expressed in diagonal form as follows:

$$\hat{\rho}_A = \sum_n \lambda^A_n |u^R_n \rangle \langle u^L_A| \langle A A, \quad (12)$$

$$A \langle u^L_n | x \rangle_A = A \langle x | u^R_n \rangle_A = \sum_k (V)_{kn} a_k(x), \quad (13)$$

$V^T V = I$. Analogously, we obtain the reduced density matrix for subsystem $B$:

$$\hat{\rho}_B = \text{tr}_A[\hat{\rho}^{AB}] = \sum_{ik} \rho^B_{ik} |b_i \rangle_B \langle b_k |, \quad (14)$$

$$\rho^B_{ik} = \sum_j e^R_{ij} e^L_{jk}, \quad (13)$$

and its diagonal form,

$$\hat{\rho}_B = \sum_n \lambda^B_n |v^R_n \rangle \langle v^L_n| \langle B B, \quad (15)$$

$$B \langle v^L_n | = \sum_j (U^{-1})^T_{jn} B \langle b_j |, \quad (17)$$

where $\lambda^B_n$ are the eigenvalues of the matrix $\rho_B = [B \langle b_i | \hat{\rho}_B | b_k \rangle_B] = [\rho^B_{ik}]$ and $U$ is the corresponding eigenvector matrix, $B \langle v^R_n | v^R_m \rangle_B = \delta_{nm}$.

Let us rewrite the matrix $\rho_A = [\rho^A_{ik}], \rho^A_{ik} = \sum_j e^R_{ij} e^L_{kj}$ and the matrix $\rho_B = [\rho^B_{ik}], \rho^B_{ik} = \sum_j e^R_{ij} e^L_{kj}$ as $\rho_A = \sum_j e^R_{ij} e^L_{kj}$.
e^R(e^L)^T and ρ_B = (e^R)^T e^L, respectively, where e^L, e^R = [e_{ij}^L, e_{ij}^R]. It is known that if C and D are square complex matrices of the same size, then the matrices CD and DC have the same eigenvalues \[32\]. We thus conclude that ρ_A and ρ_B = (e^L)^T e^R have a common set of eigenvalues. Hence, bearing in mind that ρ_B has the same eigenvalues as ρ_B, we arrive at the conclusion that the eigenvalues of ρ_A and ρ_B are identical, λ_i^A = λ_i^B = λ_i.

IV. CORRELATION MEASURES

As discussed by Moiseyev \[31\], the real and imaginary parts of the mean value of a complex-scaled operator, \[\langle \hat{Q} \rangle = \langle \psi_L | \hat{Q} | \psi_R \rangle\], give the average value of the quantity under consideration, and its uncertainty, respectively. It is easy to see that the average value of any operator acting on one of the subsystems, let it be A, is given by

\[\langle \hat{Q}_A \rangle = \langle \psi_L | \hat{Q}_A | \psi_R \rangle = \sum_{ijk} e_{kj}^{L} e_{ij}^{R} A \langle a_k^{A} | \hat{Q}_A | a_i^{A}\rangle \] \[19\]

Noting that \[\sum_j e_{kj}^{L} e_{ij}^{R} = \rho_{ik}^{A}\], we obtain

\[\langle \hat{Q}_A \rangle = \sum_{ik} \rho_{ik}^{A} A \langle a_k^{A} | \hat{Q}_A | a_i^{A}\rangle \Rightarrow \text{tr}[\rho_A \hat{Q}_A]. \] \[19\]

Let us now address the question of how to characterize the correlation in resonance states. Generally, according to the standard quantum theory, the von Neumann (vN) entropy \(S = -\text{tr}[\rho_{A,B} \ln \rho_{A,B}]\) \[38\] and the linear entropy \(S_{lin} = 1 - \text{tr}[\rho_{A,B}^2]\) \[39\] are used to quantify the degree of entanglement in composite quantum systems. In a strict mathematical sense, the values of S and \(S_{lin}\) can be given by \(S = -\ln \rho_{A,B}\) and \(S_{lin} = (1 - \rho_{A,B}) = 1 - (\hat{\rho}_{A,B})\) \[40\], where \(\langle ... \rangle\) is the conventional inner product and \(\rho\) is the identity operator from the appropriate basis set. Accordingly, in the resonance case, we have

\[S = -\langle \ln \rho_{A,B} \rangle = -\text{tr}[\rho_{A,B} \ln \rho_{A,B}] = -\sum_i \lambda_i \ln \lambda_i, \] \[20\]

and

\[S_{lin} = 1 - \langle \hat{\rho}_{A,B} \rangle = 1 - \text{tr}[\rho_{A,B}^2] = 1 - \sum_i \lambda_i^2. \] \[21\]

Thus, the real and imaginary parts of S, \((S_{lin})\) can be identified as the mean value of the operator: \(-\ln \rho_{A,B}, (1 - \rho_{A,B})\) and its uncertainty, respectively. In particular, the real part of \(\langle \hat{\rho}_{A,B} \rangle\) gives the average of the probability \(\lambda_i\), whereas the imaginary part describes its uncertainty. However, because the entropy cannot rigorously be treated as the average value of a quantal observable \[41\], the interpretation of the real part of \(S, (S_{lin})\) as the entanglement entropy of a resonance state is problematic. Despite of this fact, we call \(S\) and \(S_{lin}\) complex entropies and propose them as measures of correlation between the subsystems A and B. Thus, we identify the real and imaginary parts of \(S, (S_{lin})\) with the amount of correlation and the uncertainty of this amount, respectively. Note that the complex linear entropy of a resonance state was first introduced in \[4\].

In a way that is analogous to the standard quantum theory, the resonance state that is factorized as a product of states can be regarded as uncorrelated, this corresponds to the case in which only one eigenvalue is nonzero, \(\lambda_i = 1\), giving \(S = S_{lin} = 0\). Deviations from such a state can be characterized by the complex entropy, as discussed above.

V. EXAMPLE: TWO-BOSON SYSTEM

Thus far, we have kept our discussion quite general. As an example, we now consider a simple model system composed of two identical bosons interacting via a contact potential of strength \(g\). For the sake of simplicity, we model an external potential by \(V(x) = 0.5x^2e^{-x^2/5}\) so that the system does not exhibit any bound state. The resonance parameters of this system can be found from the following complex-scaled Hamiltonian \[42\]:

\[\hat{H}^θ = \sum_{i=1}^{2} \left[-e^{-2/θ} \partial_i^2 + v(x)e^{iθ}\right] + ve^{-iθ}\delta(x_2-x_1). \] \[22\]

Here we apply the basis function method and diagonalize the matrix Hamiltonian \(\hat{H}^θ = \langle \phi_{nm} | \hat{H}^θ | \phi_{ij}\rangle\) in a basis of permanents constructed from the one-particle orthonormal basis set,

\[\phi_{ij} = s_{ij} | \psi_i(x_1) \psi_j(x_2) + \psi_j(x_1) \psi_i(x_2)\rangle, \] \[23\]

where \(s_{ii} = 1/2\) and \(s_{ij} = 2^{-1/2}\) for \(i \neq j\). We choose as the one-particle basis the wave functions of a simple harmonic oscillator,

\[\psi_i(x) = \frac{2^{-i/2}e^{-\frac{x^2}{2\theta}}H_i(x)}{\sqrt{\theta^{\frac{i}{2}}}!}, \] \[24\]

so that the basis \[23\] is real. Hence, and because \(\hat{H}^θ\) is symmetric, then, in accordance with Section \[11\] the right and left wavefunctions of a given resonance state can be written in the same form,

\[\chi_{L,R}^θ(x_1, x_2) = \sum_{i \geq j} r_{ij} \phi_{ij}(x_1, x_2) = \sum_{ij} (e_{ij} ) \psi_i(x_1) \psi_j(x_2), \] \[25\]

with \(\sum_{ij} r_{ij}^2 = 1\), where \(\{r_{ij}\}\) is the corresponding eigenvector of \(\hat{H}^θ\), and \(\{e_{ij}\} = r_{ii} = 2^{-1/2}r_{jj}\) \((2^{-1/2}r_{ji})\) for \(i > j\) \((i < j)\). From here on we denote
\( \chi^{rez} = \chi^{L,R} \). As is easy to see, the reduced density matrix for particles 1 or 2 is

\[
\hat{\rho}_{12} = \sum_{ij} (e^2)_{ij} |\psi_i\rangle \langle \psi_j|,
\]

(26)

Because the matrix \( e \) is symmetric, its eigenvector matrix \( V (V^{-1} = V^T) \) and eigenvalues \( D = \text{diag}(d_0, d_1, \ldots) \) satisfy \( e = V \Gamma V^T \). Hence it is easy to infer that \( e^2 = V \Gamma^2 V^T \). After rewriting these formulas as

\[
(e)_{ij} = \sum_n (V)_{in} d_n (V)_{jn},
\]

(27)

and

\[
(e^2)_{ij} = \sum_n (V)_{in} d_n^2 (V)_{jn},
\]

(28)

and performing some straightforward algebra, we arrive at

\[
\chi^{rez}(x_1, x_2) = \sum_n d_n u_n(x_1) u_n(x_2),
\]

(29)

and

\[
\rho_{12}(x, x') = \langle x | \hat{\rho}_{12} | x' \rangle = \sum_n \lambda_n u_n(x) u_n(x'),
\]

(30)

where

\[
u_n(x) = \sum_k (V)_{kn} \psi_k(x),
\]

(31)

and \( \lambda_n = d_n^2 \approx u_n | u_m \rangle = \delta_{nm} \).

The resonance parameters are determined at the angle \( \theta = \theta_{opt} \) at which the eigenvalues of \( H^0 \) exhibit the most stabilized characters with respect to \( \theta \). We recall that the resonance energy \( E^{rez} \) and lifetime \( \Gamma \) are obtained from the stable eigenvalue \( W \) as \( E^{rez} = \text{Re}[W] \) and \( \Gamma = -2 \text{Im}[W] \), respectively. We find that the set of basis functions \( \{ \psi_k \} \) constructed from the 90 lowest one-particle orbitals \( \{ \psi_1, \ldots, \psi_90 \} \) is sufficiently large to obtain a good estimate of the parameters of the lowest-energy resonance state, at least over the range of \( g = 0 \) to \( g = 45 \). Moreover, in this range the optimal value of the parameter \( \theta \) is approximately \( \theta_{opt} = 0.2 \), regardless of \( g \).

We now examine the properties of the system. Let us first briefly discuss the special cases \( g = 0 \) and \( g \to \infty \), which correspond to the non-interacting case and the Tonks-Girardeau (TG) regime, respectively. In these limiting situations, the positions of the lowest resonance states are given by \( W^g=0 = 2W_0 \) and \( W^{TG} = W_0 + W_1 \), respectively, where \( W_0, W_1 \) are the lowest-energy resonance positions of the corresponding one-particle system, which we find numerically to be at \( W_0 \approx 0.411 - 0.0026I \) and \( W_1 \approx 1.014 - 0.125I \). Here we use the complex linear entropy \( S_{lin} \) as a measure of the correlation, \( S_{lin} = 1 - \text{tr} \rho_{12}^2 \). Figs. 1 and 2 show our numerical results for \( W \) and for \( S_{lin} \) as functions of \( g \), respectively. The horizontal lines in both figures indicate the results for the TG system, \( E^{rez}_{TG} \approx 1.425, \Gamma_{TG} \approx 0.254, S_{lin}^{TG} \approx 0.34 - 0.041 \), where the last result was determined from the resonance TG wavefunction constructed as

\[
\chi^{rez}_{TG}(x_1, x_2) = \text{sgn}[x_2 - x_1] \frac{1}{\sqrt{2}} \text{det}_{i=0,j=1}^{1.2} \phi_i^{rez}(x_j),
\]

(32)

where \( \phi_i^{rez} \) and \( \phi_i^{L,R} \) are the resonance orbitals of the one-particle system corresponding to \( W_0 \approx 0.411 - 0.0026I \) and \( W_1 \approx 1.014 - 0.125I \), respectively, \( \langle \phi_i^{rez} | \phi_j^{rez} \rangle \approx \delta_{ij} \). In the non-interacting case, we have \( E^{rez}_{g=0} \approx 0.822, \Gamma_{g=0} \approx 0.0104 \) and \( \chi^{rez}_{g=0}(x_1, x_2) = \phi_0^{rez}(x_1) \phi_0^{rez}(x_2) \), which gives \( S_{lin}^{g=0} = 0 \), reflecting the fact that there is no correlation between the particles. We can observe how the results obtained for finite values of \( g \) converge to those for the TG system as \( g \) is increased, which, in particular, confirms the correctness of our calculations. In fact, the system starts to exhibit the behaviour of the TG system after exceeding a value of \( g \approx 40 \). We conclude from our results that the larger
the value of \( g \), the higher the correlations produced by two bosons, which is attributed to the fact that the real part of \( S_{\text{lin}} \) increases with the increase in \( g \). As expected, the effect of changing \( g \) becomes less pronounced as \( g \) becomes larger and disappears in the limit \( g \to \infty \).

VI. CONCLUDING REMARKS

We have discussed in detail the diagonal representation of a reduced density matrix determined under the framework of the CSM. Moreover, we discussed the quantification of bipartite correlations in quantum resonance states by means of the complex entropy. We also conducted a comprehensive study of the lowest-energy resonance state of two interacting bosons trapped inside an open potential well. Among other findings, our results show the dependence of the complex linear entropy on the inter-boson interaction strength \( g \). Its real and imaginary parts have monotonically increasing behaviours as \( g \) increases and tend to constant values in the TG limit.

We hope our study will stimulate broader discussions of correlation in quantum resonance states.

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