Transition-state theory reexamined

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Two quantum systems, each described as a random-matrix ensemble, are coupled to each other via a number of transition states. Each system is strongly coupled to a large number of channels. The average transmission probability is the product of three factors describing, respectively, formation of the first system from the entrance channel, decay of the second system through the exit channel, and transport through the transition states. Each of the transition states contributes a Breit-Wigner resonance. In general, the resonances overlap.

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I. INTRODUCTION

Starting with the seminal work of Bohr and Wheeler [1], transition-state theory has played an important role in applications of many-body quantum theory to physics and chemistry (see, for instance, Refs. [2,3]). The theory aims at calculating the probability of passage through or over a barrier that separates two parts of a physical many-body system, and of the associated reaction rates. Following a suggestion in Refs. [4,5], an approach from first principles to transition-state theory has been developed in Ref. [6]. The approach describes the two parts of the system in terms of two independent random-matrix ensembles. Each of these is coupled to a number of channels that feed or deplete the system. In Ref. [6] the model was worked out explicitly for quantum tunneling through a barrier and for passage through a single transition state above the barrier (which turns into a transition-state resonance). The model has been generalized in Ref. [7] to the situation where the two parts of the system are coupled by a number of nonoverlapping transition-state resonances and where both parts are strongly coupled to a large number of channels. The present paper describes a further generalization of that model by allowing the transition-state resonances to overlap. Such generalizations may apply, for instance, to the transmission of electrons through quantum dots [8].

II. MODEL

We consider two time-reversal invariant quantum systems, each coupled to a set of scattering states. The two systems are coupled to each other via a set of k transition states. In matrix form, the Hamiltonian is

$$H = \begin{pmatrix} H_1 & V_1 & 0 \\ V_1^T & H_{\rm tr} & V_2^T \\ 0 & V_2 & H_2 \end{pmatrix}. \tag{1}$$

Here H_1 (H_2) is the real and symmetric Hamiltonian matrix governing system 1 (system 2, respectively). It acts in Hilbert space 1 (in Hilbert space 2, respectively). Both Hilbert spaces have dimension N. The real and symmetric Hamiltonian matrix $H_{\rm tr}$ acts in the transition space which has dimension k. The coupling matrices V_1 and V_2 are real and have N rows and k columns each. The upper index T denotes the transpose.

We assume that the matrices H_1 and H_2 are statistically independent members of the Gaussian orthogonal ensemble (GOE) of random matrices. Their elements are zero-centered real Gaussian random variables with second moments:

$$\langle (H_1)_{\mu_1\mu_1'} (H_1)_{\mu_2\mu_2'} \rangle = \frac{\lambda^2}{N} (\delta_{\mu_1\mu_2}\delta_{\mu_1'\mu_2'} + \delta_{\mu_1\mu_2'}\delta_{\mu_1'\mu_2}),$$
$$\langle (H_2)_{\nu_1\nu_1'} (H_2)_{\nu_2\nu_2'} \rangle = \frac{\lambda^2}{N} (\delta_{\nu_1\nu_2}\delta_{\nu_1'\nu_2'} + \delta_{\nu_1\nu_2'}\delta_{\nu_1'\nu_2}). \tag{2}$$

The angular brackets denote the ensemble average. The parameter λ defines the ranges of the two spectra. All indices labeled μ and μ' run from 1 to N; those labeled ν and ν' run from $N+k+1$ to $2N+k$. Elements of the matrix $H_{\rm tr}$ carry indices m, m', n, and n' that range from $N+1$ to $N+k$. We eventually consider the limit $N \to \infty$, keeping k fixed. We assume that the k eigenvalues E_m of $H_{\rm tr}$ are all located near the centers of the spectra of H_1 and H_2.

We show in the Appendix that we may always write V_1 and V_2 in the following forms:

$$(V_1)_{\mu m} = \sum_{m'} (O_1)_{\mu m'} \mathcal{V}_{1,m'} (O_{\rm tr,1})_{mm'},$$
$$(V_2)_{\nu m} = \sum_{m'} (O_2)_{\nu m'} \mathcal{V}_{2,m'} (O_{\rm tr,2})_{mm'}. \tag{3}$$

Here O_1 and O_2 are orthogonal matrices of dimension N, and $O_{\rm tr,1}$ and $O_{\rm tr,2}$ are orthogonal matrices of dimension k. Equations (3) show that the rows of the matrices V_1 and V_2

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are linear superpositions of the k vectors $Z_{1,m'}$ and $Z_{2,m'}$ in transition space, with components

$$(Z_{1,m'})_m = \mathcal{V}_{1,m'}(O_{\mathrm{tr},1})_{mm'},$$
$$(Z_{2,m'})_m = \mathcal{V}_{2,m'}(O_{\mathrm{tr},2})_{mm'}, \tag{4}$$

and with lengths $|\mathcal{V}_{1m'}|$ and $|\mathcal{V}_{2m'}|$, respectively. The arguments in Ref. [6] show that for all m', $|\mathcal{V}_{1,m'}|$ and $|\mathcal{V}_{2,m'}|$ must be small compared to λ.

Each of the two GOE Hamiltonians is coupled to a set of open channels labeled, respectively, a, a', a'', etc., for H_1 and b, b', b'', etc., for H_2. The real coupling matrix elements are labeled $W_{1,a\mu}$ and $W_{2,b\nu}$, respectively. These obey

$$\sum_\mu W_{1,a\mu}W_{1,a'\mu} = \delta_{aa'}v_{1,a}^2,$$
$$\sum_\nu W_{2,b\nu}W_{2,b'\nu} = \delta_{bb'}v_{2,b}^2. \tag{5}$$

The relations (5) define the coupling strengths $v_{1,a}^2$ and $v_{2,b}^2$. The Kronecker deltas rule out direct (i.e., nonresonant) scattering processes $a \to a'$ and $b \to b'$ [9]. We define the $N \times N$ width matrices Γ_1 and Γ_2 as

$$(\Gamma_1)_{\mu\mu'} = 2\pi\sum_a W_{1,a\mu}W_{1,a\mu'},$$
$$(\Gamma_2)_{\nu\nu'} = 2\pi\sum_b W_{2,b\nu}W_{2,b\nu'}, \tag{6}$$

and, in analogy to Eq. (1), the total width matrix Γ as

$$\Gamma = \begin{pmatrix} \Gamma_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Gamma_2 \end{pmatrix}. \tag{7}$$

With E the total energy of the system, the inverse of the propagator matrix of the system is

$$D(E) = \mathbf{E} - H + (i/2)\Gamma. \tag{8}$$

Here and in what follows, $\mathbf{E}$ stands for the product of the variable E and the unit matrix in the space under consideration.

There are two types of scattering processes: (i) backscattering from channel a to channel a' (or from channel b to channel b') on the same side of the transition region, and (ii) transmission from channel a through the transition region to channel b or vice versa. The elements of the scattering matrix $S(E)$ for backscattering are given by

$$S_{aa'}(E) = \delta_{aa'} - 2i\pi\sum_{\mu\mu'} W_{1,a\mu}(D^{-1}(E))_{\mu\mu'}W_{1,a'\mu'},$$
$$S_{bb'}(E) = \delta_{bb'} - 2i\pi\sum_{\nu\nu'} W_{2,b\nu}(D^{-1}(E))_{\nu\nu'}W_{2,b'\nu'}, \tag{9}$$

those for transmission through the transition region are given by

$$S_{ab}(E) = -2i\pi\sum_{\mu\nu} W_{1,a\mu}(D^{-1}(E))_{\mu\nu}W_{2,b\nu},$$
$$S_{ba}(E) = -2i\pi\sum_{\nu\mu} W_{2,b\nu}(D^{-1}(E))_{\nu\mu}W_{1,a\mu}. \tag{10}$$

It is easy to check that the S matrix is unitary and symmetric.

III. MANY STRONGLY COUPLED CHANNELS

We calculate $\langle S_{ab}(E)\rangle$ and $\langle|S_{ab}(E)|^2\rangle$ by averaging over both H_1 and H_2. We expand $(D^{-1}(E))_{\mu\nu}$ in powers of V_1 and V_2. We resum the resulting series. To write the result in compact form, we define the Green functions

$$G_1(E) = [\mathbf{E} - H_1 + (i/2)\Gamma_1]^{-1},$$
$$G_2(E) = [\mathbf{E} - H_2 + (i/2)\Gamma_2]^{-1},$$
$$G_{\mathrm{tr}}(E) = \big[\mathbf{E} - H_{\mathrm{tr}} - V_1^T G_1(E)V_1 - V_2^T G_2(E)V_2\big]^{-1}. \tag{11}$$

With these definitions, the first of Eqs. (10) becomes

$$S_{ab}(E) = -2i\pi\sum_{\mu\nu} W_{1,a\mu}\big[G_1(E)V_1G_{\mathrm{tr}}(E)V_2^T G_2(E)\big]_{\mu\nu}W_{2,b\nu}. \tag{12}$$

Equations (11) show that $G_1(E)$, $G_2(E)$, and $G_{\mathrm{tr}}(E)$ are statistically correlated. Therefore, it is not possible, in general, to calculate $\langle S_{ab}(E)\rangle$ and $\langle|S_{ab}(E)|^2\rangle$ analytically. Complete analytical expressions can be obtained, however, if the numbers of channels strongly coupled to H_1 and to H_2 are both large compared to unity. That is the case we consider. To quantify that condition we consider backscattering for a closed transition space defined by putting $V_1 = 0 = V_2$ in Eq. (1). Equations (9) then define two backscattering matrices $S_1(E)$ and $S_2(E)$, given by

$$(S_1(E))_{aa'} = \delta_{aa'} - 2i\pi\sum_{\mu\mu'} W_{1,a\mu}G_1(E)_{\mu\mu'}W_{1,a'\mu'},$$
$$(S_2(E))_{bb'} = \delta_{bb'} - 2i\pi\sum_{\nu\nu'} W_{2,b\nu}G_2(E)_{\nu\nu'}W_{2,b'\nu'}. \tag{13}$$

These depend, respectively, only on H_1 (only on H_2). The ensemble averages of $(S_1(E))_{aa'}$ and $(S_2(E))_{bb'}$ are diagonal. That follows [9] from Eqs. (5). The average values define the transmission coefficients

$$T_{1,a} = 1 - |\langle(S_1)_{aa}\rangle|^2\ ,\ T_{2,b} = 1 - |\langle(S_2)_{bb}\rangle|^2\ . \tag{14}$$

We assume $\sum_a T_{1,a} \gg 1$ and $\sum_b T_{2,b} \gg 1$. The strong inequalities imply that terms of order $1/\sum_a T_{1,a}$ and $1/\sum_b T_{2,b}$ are negligible compared to terms of order unity. We calculate the leading-order terms in an asymptotic expansion of $\langle S_{ab}(E)\rangle$ and of $\langle|S_{ab}(E)|^2\rangle$ in inverse powers of $\sum_a T_{1,a}$ and $\sum_a T_{2,b}$.

For $\sum_a T_{1,a} \gg 1$ and $\sum_b T_{2,b} \gg 1$, the arguments in Ref. [6] show that in the expression for $G_{\mathrm{tr}}(E)$ in Eq. (11) we may replace $G_1(E)$ and $G_2(E)$ by their average values. With E close to the centers of the spectra of H_1 and H_2, these averages are given by

$$\langle G_1(E)\rangle_{\mu\mu'} = -(i/\lambda)\delta_{\mu\mu'}, \quad \langle G_2(E)\rangle_{\nu\nu'} = -(i/\lambda)\delta_{\nu\nu'}. \tag{15}$$

Insertion into the last Eq. (11) and use of the definitions (4) gives

$$G_{\mathrm{tr}}(E) = \big(\mathbf{E} - H_{\mathrm{tr}} + iV_1^TV_1/\lambda + iV_2^TV_2/\lambda\big)^{-1} = \left(\mathbf{E} - H_{\mathrm{tr}} + i\sum_{j=1}^{2}\sum_m Z_{j,m}^T Z_{j,m}/\lambda\right)^{-1}. \tag{16}$$

We note that Eq. (16) does not contain any random elements. Substituting $G_{\rm tr}(E)$ given by Eq. (16) into Eq. (12) yields an expression for $S_{ab}(E)$ that depends upon H_1 (H_2) only via the factor $G_1(E)$ [the factor $G_2(E)$, respectively]. That allows us to calculate $\langle S_{ab}(E)\rangle$ and $\langle|S_{ab}(E)|^2\rangle$ analytically.

IV. AVERAGE TRANSMISSION AMPLITUDE

We calculate $\langle S_{ab}(E)\rangle$ by averaging separately the factors that depend upon H_1 and on H_2. For the first of these we use Eqs. (3) and the definition of the vectors $Z_{1,m'}$ in Eqs. (4) to write

$$\sum_{\mu} W_{1,a\mu}(G_1(E)V_1)_{\mu m} = \sum_{\mu\mu' m'} W_{1,a\mu}(G_1(E))_{\mu\mu'}(O_1)_{\mu' m'}(Z_{1,m'})_m. \tag{17}$$

We define

$$\tilde{H}_1 = O_1^T H_1 O_1, \quad \tilde{W}_{1,a\mu} = \sum_{\mu'} W_{1,a\mu'}(O_1)_{\mu'\mu},$$
$$\tilde{G}(E) = O_1^T G_1(E) O_1. \tag{18}$$

Then expression (17) takes the form

$$\sum_{\mu m'} \tilde{W}_{1,a\mu}(\tilde{G}_1(E))_{\mu m'}(Z_{1,m'})_m. \tag{19}$$

We observe that, with H_1, the matrix $\tilde{H}_1$ is also a member of the GOE and that the coefficients $\tilde{W}_{a\mu}$ also obey the first of Eqs. (5). We use the first of Eqs. (15) for $\tilde{G}_1(E)$. For expression (19) that gives

$$-\frac{i}{\lambda}\sum_{m'} \tilde{W}_{1,am'}(Z_{1,m'})_m. \tag{20}$$

The sum over m' has k terms. The first of Eqs. (5) shows that, for $N \to \infty$, $\tilde{W}_{a\mu}$ is inversely proportional to $1/\sqrt{N}$. It follows that, for fixed k and $N \to \infty$, expression (20) vanishes. Thus,

$$\langle S_{ab}(E)\rangle = 0. \tag{21}$$

The same conclusion is reached when we consider, instead of expression (17), the term $\sum_\nu [V_2^T G_2(E)]_{m\nu} W_{2,b\nu}$ in Eq. (12).

V. AVERAGE TRANSMISSION PROBABILITY

With $\langle S_{ab}(E)\rangle = 0$, the average probability for transmission from channel a to channel b is given by

$$P_{ab}(E) = \langle|S_{ab}(E)|^2\rangle. \tag{22}$$

The average is over both H_1 and H_2. We use Eq. (16) in Eq. (12). We use the transformation leading to Eq. (19) and the corresponding transformation for the term containing $G_2(E)$. We calculate

$$X_{1a,m'm''} = 2\pi\left\langle \sum_{\mu} \tilde{W}_{1,a\mu}\tilde{G}_1(E)_{\mu m'} \sum_{\mu'} \tilde{W}_{1,a\mu'}\tilde{G}_1^*(E)_{\mu' m''}\right\rangle,$$
$$X_{2b,m'm''} = 2\pi\left\langle \sum_{\nu} \tilde{G}_2(E)_{m'\nu}\tilde{W}_{2,b\nu} \sum_{\nu'} \tilde{G}_2^*(E)_{m''\nu'}\tilde{W}_{2,b\nu'}\right\rangle. \tag{23}$$

The first (second) set of angular brackets denotes the average over H_1 (over H_2, respectively). A slight generalization of the argument used in the Appendix of Ref. [6] shows that in the limit of many strongly coupled channels we have

$$X_{1a,m'm''} = \delta_{m'm''}\frac{1}{\lambda}\frac{T_{1,a}}{\sum_{a'} T_{1,a'}},$$
$$X_{2b,m'm''} = \delta_{m'm''}\frac{1}{\lambda}\frac{T_{2,b}}{\sum_{b'} T_{2,b'}}. \tag{24}$$

The Kronecker deltas are due to the orthogonal invariance of the two ensembles. Using Eqs. (24) in the expression for $|\langle S_{ab}\rangle|^2$, we obtain for the average transmission probability P_{ab} defined in Eq. (22) the expression

$$P_{ab}(E) = \frac{T_{1,a}}{\sum_{a'} T_{1,a'}} Y \frac{T_{2,b}}{\sum_{b'} T_{2,b'}}, \tag{25}$$

where

$$Y = \sum_{mn}\left|\sum_{m'n'}(z_{1,m})_{m'}(G_{\rm tr}(E))_{m'n'}(z_{2,n})_{n'}\right|^2, \tag{26}$$

where $(G_{\rm tr}(E))$ is given by Eq. (16) and where

$$z_{1,m} = Z_{1,m}/\sqrt{\lambda}\,, \quad z_{2,m} = Z_{2,m}/\sqrt{\lambda}\,. \tag{27}$$

Equation (25) gives the average transmission probability as the product of three factors. The first (last) factor is the probability to enter (leave) space 1 (space 2) via channel a (via channel b, respectively). The fact that $P_{ab}(E)$ factorizes and the forms of the first and last factors are all due to the statistical properties of H_1 and H_2 and to the assumptions $\sum_a T_{1,a} \gg 1$ and $\sum_b T_{2,b} \gg 1$. That is seen by comparing Eq. (25) with the result of the theory of compound-nucleus scattering [9]. There one uses a scattering matrix of the form of $(S_1(E))_{aa'}$ as in Eqs. (13), with H_1 being a member of the GOE. For $a \neq a'$, for $N \to \infty$, and for $\sum_{a''} T_{1,a''} \gg 1$, the resulting expression for $\langle|(S_1(E))_{aa'}|^2\rangle$ factorizes and has the form [10]

$$\langle|(S_1(E))_{aa'}|^2\rangle = T_{1,a}\frac{T_{1,a'}}{\sum_{a''} T_{1,a''}}, \quad a \neq a'. \tag{28}$$

That form is known as "independence of formation and decay of the compound nucleus," with $T_{1,a}$ interpreted as the probability of compound-nucleus formation, and the second factor interpreted as the relative probability of compound-nucleus decay into channel a'. Equation (25) differs in form from Eq. (28) in that it contains two factors, each denoting a relative probability. That is a consequence of the symmetry of $S_{ab}(E)$ in Eqs. (10) under the operation $a \leftrightarrow b$.

The factor Y in Eq. (26) describes transport through the transition space. It does not depend on the couplings of system 1 and system 2 to the channels. We show presently that this apparent independence is the result of the assumptions $\sum_a T_{1,a} \gg 1$ and $\sum_b T_{2,b} \gg 1$. The factor Y is the sum of squares of amplitudes, each of which bears a close formal analogy to the inelastic parts of the S matrices in Eqs. (13). Indeed, the transition space is entered from space 1 through "channel" m and left for space 2 through "channel" n via the vectors $z_{1,m}$ and $z_{2,n}$, respectively. The elements $(z_{1,m})_{m'}$ and $(z_{2,n})_{m'}$ are analogs of the amplitudes $\sqrt{2\pi}W_{1,a\mu}$ and

$\sqrt{2\pi}W_{2,bv}$ in Sec. II. All have dimension (energy)$^{1/2}$. Propagation within the transition space is governed by the effective Hamiltonian

$$\mathcal{H}_{\rm eff} = H_{\rm tr} - i\sum_{j=1}^{2}\sum_{m} z_{j,m}^{T} z_{j,m}, \tag{29}$$

which differs from $H_{\rm tr}$ because it accounts for the coupling to spaces 1 and 2. The coupling term has the same form and plays the same role as the width matrices in Eqs. (6) and (8). It differs from the width term in Eq. (8) by a factor of 2. While the width matrix in Eq. (8) is due to the free propagator in channel space, the coupling term in Eq. (29) is a remnant of the propagators $G_1(E)$ and $G_2(E)$ in spaces 1 and 2, respectively. Propagation in these spaces is subject to the coupling to the channels. In the limits $\sum_a T_{1,a} \gg 1$ and $\sum_b T_{2,b} \gg 1$, $G_1(E)$ and $G_2(E)$ take the forms (15) wherein all explicit reference to the channels disappears. Nevertheless, the coupling to the channels leaves us with the abovementioned factor of 2. Equation (26) shows that the factor Y is determined entirely by the dynamics in transition space. That is a consequence of the orthogonal invariance of H_1 and H_2. Using the definitions (27), (4), and (3) and the orthogonality of the matrices O_1 and O_2, we can rewrite Y identically as

$$Y = (1/\lambda^2)\sum_{\mu\nu}\left|\sum_{m'n'}(V_1)_{\mu m'}(G_{\rm tr})_{m'n'}(V_2)_{\nu n'}\right|^2. \tag{30}$$

Here, $G_{\rm tr}(E)$ is given by the first of Eqs. (16). Equations (30) and (16) relate Y to the matrices V_1 and V_2 introduced originally in our model. They generalize Eq. (32) and the second of Eqs. (31) of Ref. [6] to the case of several transition states and offer an intuitive understanding of the transmission process.

The Hamiltonian $\mathcal{H}_{\rm eff}$ is complex symmetric and can be diagonalized by a complex orthogonal matrix $\mathcal{O}$,

$$(\mathcal{H}_{\rm eff})_{mn} = \sum_{l=1}^{k}\mathcal{O}_{ml}\mathcal{E}_l\mathcal{O}_{nl}. \tag{31}$$

The k complex eigenvalues $\mathcal{E}_l$, $l = 1, \ldots, k$, obey $\mathrm{Im}(\mathcal{E}_l) < 0$ for all l. For $j = 1$ and 2, we define amplitudes

$$\zeta_{j,ml} = \sum_{m'}(z_{j,m})_{m'}\mathcal{O}_{m'l} \tag{32}$$

and obtain

$$Y = \sum_{mn}\left|\sum_{l}\zeta_{1,ml}\frac{1}{E-\mathcal{E}_l}\zeta_{2,nl}\right|^2. \tag{33}$$

Insertion of that into Eq. (25) gives our final result,

$$P_{ab}(E) = \frac{T_{1,a}}{\sum_{a'}T_{1,a'}}\sum_{mn}\left|\sum_{l}\zeta_{1,ml}\frac{1}{E-\mathcal{E}_l}\zeta_{2,nl}\right|^2\frac{T_{2,b}}{\sum_{b'}T_{2,b'}}. \tag{34}$$

The total transmission probability is given by

$$\sum_b P_{ab}(E) = \frac{T_{1,a}}{\sum_{a'}T_{1,a'}}\sum_{mn}\left|\sum_{l}\zeta_{1,ml}\frac{1}{E-\mathcal{E}_l}\zeta_{2,nl}\right|^2. \tag{35}$$

In Eqs. (34) and (35), each transition state contributes to transmission through the transition space of a Breit-Wigner resonance with complex resonance energy $\mathcal{E}_l = \varepsilon_l - i\gamma_l$. The resonance energies are ordered by putting $\varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_k$. Equations (15) may be used in $G_{\rm tr}$ only if all ε_l are close to the centers $E = 0$ of the spectra of H_1 and H_2. An equivalent assumption was formulated in Sec. II.

To interpret Eqs. (34) and (35), we consider two extreme cases. (i) The k resonances are isolated so that $\varepsilon_l - \varepsilon_{l-1} \gg \gamma_l, \gamma_{l-1}$ for all $l = 2, \ldots, k$. Then Y reduces to

$$Y = \sum_{mnl}\left|\zeta_{1,ml}\frac{1}{E-\mathcal{E}_l}\zeta_{2,nl}\right|^2. \tag{36}$$

Transmission is described by a sum of Lorentzians. That is somewhat similar to the case considered in Ref. [7] where simplifying statistical assumptions on the matrices V_1 and V_2 are used. These prevent the resonances from overlapping and cause all resonances to have the same partial and total widths. (ii) All resonances overlap so that $\gamma_l, \gamma_{l-1} \leqslant \varepsilon_l - \varepsilon_{l-1}$ for all l. Then

$$Y = \sum_{mn}\sum_{ll'}\zeta_{1,ml}\frac{1}{E-\mathcal{E}_l}\zeta_{2,nl}\zeta^*_{1,ml'}\frac{1}{E-\mathcal{E}^*_{l'}}\zeta^*_{2,nl'}, \tag{37}$$

with nonnegligible interference terms between pairs $l \neq l'$ of resonances. The values of Y for cases (i) and (ii) may differ substantially. The actual physical situation may lie anywhere between cases (i) and (ii). It seems that only case (i) has so far been considered in the literature. The presence or absence of interference terms could be tested experimentally using a beam with variable mean energy E and band width $\delta E < \varepsilon_l - \varepsilon_{l-1}$.

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APPENDIX

We derive the first of Eqs. (3), and the second follows analogously. The matrices $V_1V_1^T$ and $V_1^TV_1$ have, respectively, dimensions N and k. Both are real and symmetric. Thus, $V_1V_1^T$ and $V_1^TV_1$ are diagonalized by orthogonal matrices O_1 of dimension N and and $O_{{\rm tr},1}$ of dimension k, respectively, so that

$$\begin{aligned}\left(V_1V_1^T\right)_{\mu\mu'} &= \sum_{s=1}^{k}(O_1)_{\mu s}\mathcal{V}_s^2(O_1)_{\mu' s},\\ \left(V_1^TV_1\right)_{mm'} &= \sum_{t=1}^{k}(O_{{\rm tr},1})_{mt}\mathcal{W}_t^2(O_{{\rm tr},1})_{m't}.\end{aligned} \tag{A1}$$

Both matrices $V_1V_1^T$ and $V_1^TV_1$ are positive semidefinite. Therefore, all eigenvalues are positive or zero. In Eqs. (A1), that fact is taken into account by writing the eigenvalues as squares of real numbers. The rank of V_1 is k. Therefore, at most k eigenvalues of $V_1V_1^T$ differ from zero. That fact is indicated in the summation over s in the first of Eqs. (A1). In the identity $V_1(V_1^TV_1) = (V_1V_1^T)V_1$ we replace the contents of the round brackets by the right-hand sides of Eqs. (A1).

After some simple matrix algebra, the identity takes the form

$$\left[O_1^T V_1 O_{\mathrm{tr},1}\right]_{\mu m} \mathcal{W}_m^2 = \mathcal{V}_\mu^2 \left[O_1^T V_1 O_{\mathrm{tr},1}\right]_{\mu m}. \tag{A2}$$

Equation (A2) implies $\mathcal{W}_m^2 = \mathcal{V}_m^2$ for all $m = 1, \ldots, k$ and $[O_1^T V_1 O_{\mathrm{tr},1}]_{\mu m} \propto \delta_{\mu m}$. Insertion of that relation into the first of Eqs. (A1) shows that the proportionality constant is $\mathcal{V}_m$, so that $[O_1^T V_1 O_{\mathrm{tr},1}]_{\mu m} = \mathcal{V}_m \delta_{\mu m}$. That yields the first of Eqs. (3).

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