1 Green's symmetrical theorem

In Cartesian coordinates $(x^1, \ldots, x^n)$ Green's symmetrical theorem reads

$$\int_V (\mathcal{U}\nabla^2\mathcal{V} - \mathcal{V}\nabla^2\mathcal{U})dV = \int_S (\mathcal{U}\nabla\mathcal{V} - \mathcal{V}\nabla\mathcal{U}) \cdot d\mathbf{S}, \tag{1}$$

where $\mathcal{U} = \mathcal{U}(x^1, \ldots, x^n)$ and $\mathcal{V}(x^1, \ldots, x^n)$ are arbitrary (complex) functions that are at least twice differentiable, and S is a surface enclosing the region V. Let the surface S be defined by

$$R(x^1, \ldots, x^n) = C. \tag{2}$$

Let the coordinates $q^1, \ldots, q^{n-1}$ be orthogonal to R, i.e., let the fundamental tensor for the coordinate system $(R, q^1, \ldots q^{n-1})$ be block diagonal:

$$g_{R,q_i} = g_{q_i,R} = 0, \; i = 1, \ldots, n-1. \tag{3}$$

Thus, for the determinant (g) of the fundamental tensor we have

$$g = g_{R,R}|g_{q_i,q_j}|. \tag{4}$$

For the surface element of integration $d\mathbf{S}$ we have

$$d\mathbf{S} = \frac{1}{|\mathbf{n}|}\mathbf{n}|g_{q_i,q_j}|^{\frac{1}{2}} dq^1 \ldots dq^{n-1}, \tag{5}$$

where the components n_i of the normal $\mathbf{n}$ to the surface are given by

$$n_i = \frac{\partial R}{\partial x^i}. \tag{6}$$

For the length of $\mathbf{n}$ we have (using Einstein summation convention, and the inverse fundamental tensor for Cartesian coordinates $g^{ij} = \delta^{ij}$)

$$|\mathbf{n}| = (n_i g^{ij} n_j)^{\frac{1}{2}} = (g^{R,R})^{\frac{1}{2}} = g_{R,R}^{-\frac{1}{2}}. \tag{7}$$

Combining the last four equations we find

$$d\mathbf{S} = \mathbf{n} g^{\frac{1}{2}} dq^1 \ldots dq^{n-1}. \tag{8}$$

We can now write the first surface term in tensor form

$$\int_S \mathcal{U}\nabla\mathcal{V} \cdot d\mathbf{S} = \int_S \mathcal{U}\mathbf{n} \cdot (\nabla\mathcal{V}) g^{\frac{1}{2}} dq^1 \ldots dq^{n-1} \tag{9}$$

$$= \int_S \mathcal{U} n_i g^{ij} \frac{\partial \mathcal{V}}{\partial x^j} g^{\frac{1}{2}} dq^1 \ldots dq^{n-1} \tag{10}$$

Note that the factor $n_i g^{ij} \frac{\partial \mathcal{V}}{\partial x^j}$ is a scalar and we can write it in the new coordinate system

$$(x^{1'}, \ldots, x^{n'}) = (R, q^1, \ldots, q^{n-1}) \tag{11}$$

for which the fundamental tensor is block diagonal and for which we have

$$n_{i'} = \frac{\partial R}{\partial x^{i'}} = \delta^1_{i'} \tag{12}$$

giving

$$n_{i'} g^{i'j'} \frac{\partial \mathcal{V}}{\partial x^{j'}} = g^{RR} \frac{\partial \mathcal{V}}{\partial R}. \tag{13}$$

Thus Green's symmetrical theorem can be written as

$$\int_V (\mathcal{U}\nabla^2\mathcal{V} - \mathcal{V}\nabla^2\mathcal{U})dV = \int_S (\mathcal{U}\frac{\partial}{\partial R}\mathcal{V} - \mathcal{V}\frac{\partial}{\partial R}\mathcal{U}) g^{R,R} g^{\frac{1}{2}} dq^1 \ldots dq^{n-1}. \tag{14}$$

2 The Wronskian

We define the Wronskian

$$\mathcal{W}(\mathcal{U},\mathcal{V}) \equiv \int_S (\mathcal{U}\frac{\partial}{\partial R}\mathcal{V} - \mathcal{V}\frac{\partial}{\partial R}\mathcal{U})\mu^{-1}g^{\frac{1}{2}}dq^1 \dots dq^{n-1} \tag{15}$$

where $\mu \equiv g_{R,R}$, and the kinetic energy operator

$$\hat{T} \equiv -\frac{\hbar^2}{2}\nabla^2 \tag{16}$$

Introducing bracket notation without complex conjugation in the bra,

$$\langle\mathcal{U}|\mathcal{V}\rangle \equiv \int_V \mathcal{U}\mathcal{V}dV \tag{17}$$

we can write Green's symmetrical theorem as

$$\langle\mathcal{U}|\hat{H} - E|\mathcal{V}\rangle - \langle\mathcal{V}|\hat{H} - E|\mathcal{U}\rangle = -\frac{\hbar^2}{2}\mathcal{W}(\mathcal{U},\mathcal{V}) \tag{18}$$

In order to expand the functions $\mathcal{U}$ and $\mathcal{V}$ we introduce and orthogonal set of functions $\phi_i(\mathbf{q})$ on S

$$\int_S \phi_i(\mathbf{q})\phi_j(\mathbf{q})dq^1 \dots dq^{n-1} = \delta_{ij} \tag{19}$$

The function $\mathcal{U}$ can now be expanded as

$$\mathcal{U}(R,\mathbf{q}) = \sum_i \mu^{\frac{1}{2}}g^{-\frac{1}{4}}\phi_i(\mathbf{q})u_i(R) \tag{20}$$

and similarly for $\mathcal{V}$. Substituting these expansions into the expression for the Wronskian gives

$$\mathcal{W}(\mathcal{U},\mathcal{V}) = \sum_i u_i(R)\frac{\partial}{\partial R}v_i(R) - v_i(R)\frac{\partial}{\partial R}u_i(R). \tag{21}$$

Note that the term involving the derivative of $\mu^{\frac{1}{2}}g^{-\frac{1}{4}}$ cancels. In vector notation

$$\mathbf{f} = [f_1(R)\dots f_n(R)]^T \tag{22}$$

we get

$$\mathcal{W}(\mathbf{f},\mathbf{g}) \equiv \mathcal{W}(\mathcal{U},\mathcal{V}) = \mathbf{f}^T\mathbf{g}' - \mathbf{f}'^T\mathbf{g}. \tag{23}$$

3 Properties of the Wronskian

The Wronskian depends on the functions $\mathcal{U}$ and $\mathcal{V}$ and on the choice of the surface S. Suppose the functions f and g are solutions of the following second order differential equations

$$\frac{\partial^2}{\partial R^2}\mathbf{u} = W(R)\mathbf{u} \tag{24}$$

$$\frac{\partial^2}{\partial R^2}\mathbf{g} = W(R)\mathbf{g}, \tag{25}$$

then

$$\frac{\partial}{\partial R}\mathcal{W}(\mathbf{u},\mathbf{g}) = \mathbf{u}^T\mathbf{g}'' - \mathbf{u}''^T\mathbf{g} \tag{26}$$

$$= \mathbf{u}^T W\mathbf{g} - (W\mathbf{u})^T\mathbf{g} \tag{27}$$

$$= \mathbf{u}^T(W - W^T)\mathbf{g} \tag{28}$$

Thus, if $W = W^T$, then $\mathcal{W}(\mathbf{u}, \mathbf{v})$ is constant.

The Wronskian is bilinear and anti-symmetric

$$\mathcal{W}(\mathbf{u}, \mathbf{v}) = -\mathcal{W}(\mathbf{v}, \mathbf{u}) \tag{29}$$

$$\mathcal{W}(\sum_i \mathbf{u}_i c_i, \sum_j \mathbf{v}_j d_j) = \sum_{i,j} c_i \mathcal{W}(\mathbf{u}_i, \mathbf{v}_j) d_j \tag{30}$$

4 Matrix notation

Let $\mathbf{U}$ denote the matrix

$$\mathbf{U} = [\mathbf{u}_1 \ldots \mathbf{u}_n], \tag{31}$$

where each column defines a function. The associated n functions are denoted as the row vector $\mathcal{U} = \{\mathcal{U}_1, \ldots, \mathcal{U}_n\}$. Defining a Wronskian *matrix* for two sets of functions

$$\mathcal{W}(\mathbf{U}, \mathbf{V})_{i,j} \equiv \mathcal{W}(\mathbf{U}_i, \mathbf{V}_j) \tag{32}$$

we can write

$$\mathcal{W}(\mathbf{U}, \mathbf{V}) = \mathbf{U}^T \mathbf{V}' - \mathbf{U}'^T \mathbf{V}. \tag{33}$$

This gives

$$\mathcal{W}(\mathbf{U}, \mathbf{V}) = -\mathcal{W}(\mathbf{V}, \mathbf{U})^T \tag{34}$$

and

$$\mathcal{W}(\mathbf{UP}, \mathbf{VQ}) = \mathbf{P}^T \mathcal{W}(\mathbf{U}, \mathbf{V}) \mathbf{Q} \tag{35}$$

if $\mathbf{P}$ and $\mathbf{Q}$ are constant matrices. Note that

$$\mathcal{W}(\mathbf{U}, \mathbf{U}) = -\mathcal{W}(\mathbf{U}, \mathbf{U})^T \tag{36}$$

only implies that the diagonal of this Wronskian is zero, and but not necessarily the entire matrix.

We also define a matrix of integrals

$$\langle\!\langle \mathcal{U} | \hat{T} | \mathcal{V} \rangle\!\rangle_{ij} \equiv \langle \mathcal{U}_i | \hat{T} | \mathcal{V}_j \rangle. \tag{37}$$

In matrix notation Green's theorem becomes

$$\langle\!\langle \mathcal{U} | \hat{T} | \mathcal{V} \rangle\!\rangle - \langle\!\langle \mathcal{V} | \hat{T} | \mathcal{U} \rangle\!\rangle^T = -\frac{\hbar^2}{2} \mathcal{W}(\mathbf{U}, \mathbf{V}) \tag{38}$$

We will call the sets of functions $\{\mathcal{U}, \mathcal{V}\}$ canonical if

$$\mathcal{W}(\mathbf{U}, \mathbf{U}) = \mathcal{W}(\mathbf{V}, \mathbf{V}) = \mathbf{0} \tag{39}$$

$$\mathcal{W}(\mathbf{U}, \mathbf{V}) = c\mathbf{I} \tag{40}$$

and $c \neq 0$. If $\{\mathcal{U}, \mathcal{V}\}$ is canonical then $\{\mathcal{U}\mathbf{A}^{-T}, \mathcal{V}\mathbf{A}\}$ is also canonical.

5 K, S, and T matrices

Let $\mathcal{F}$ and $\mathcal{G}$ be sets of real functions with

$$\mathcal{W}(\mathcal{F}, \mathcal{F}) = \mathcal{W}(\mathcal{G}, \mathcal{G}) = \mathbf{0} \tag{41}$$

and

$$\mathcal{W}(\mathcal{F}, \mathcal{G}) = \mathbf{I}. \tag{42}$$

The general form of the wave function is

$$\Psi = \mathcal{U} + \mathcal{V}\mathbf{E} \tag{43}$$

with $\{\mathcal{U}, \mathcal{V}\}$ canonical and

$$\mathcal{W}(\mathcal{U}, \mathcal{V}) \equiv c_E \mathbf{I} \tag{44}$$

The definitions of the **K**, **S**, and **T** matrices are

$$\begin{aligned}
\Psi_K &= \mathcal{F} + \mathcal{G}\mathbf{K} & (45)\\
\Psi_S &= (\mathcal{F} - i\mathcal{G}) + (\mathcal{F} + i\mathcal{G})\mathbf{S} = \mathcal{F}(\mathbf{I} + \mathbf{S}) + \mathcal{G}(-i\mathbf{I} + i\mathbf{S}) & (46)\\
\Psi_T &= \mathcal{F} + (\mathcal{F} + i\mathcal{G})\mathbf{T} = \mathcal{F}(\mathbf{I} + \mathbf{T}) + \mathcal{G}i\mathbf{T} & (47)
\end{aligned}$$

The Wronskians are

$$\begin{aligned}
c_K &= 1 & (48)\\
c_S &= 2i & (49)\\
c_T &= i & (50)
\end{aligned}$$

In general we can write

$$\Psi = (\mathcal{U} + \mathcal{V}\mathbf{E})\mathbf{X} \tag{51}$$

where $\{\mathcal{U}, \mathcal{V}\}$ is a canonical set. We can solve for the matrix **E** as follows:

$$\begin{aligned}
\mathcal{W}(\mathcal{U}, \Psi) &= \mathcal{W}(\mathcal{U}, \mathcal{V})\mathbf{E}\mathbf{X} & (52)\\
\mathcal{W}(\mathcal{V}, \Psi) &= \mathcal{W}(\mathcal{V}, \mathcal{U})\mathbf{X} & (53)
\end{aligned}$$

thus,

$$\mathbf{E} = \mathcal{W}(\mathcal{U}, \mathcal{V})^{-1}\mathcal{W}(\mathbf{U}, \Psi)\mathbf{X}^{-1} \tag{54}$$

together with

$$\mathbf{X} = \mathcal{W}(\mathcal{U}, \mathcal{V})^{-1}\mathcal{W}(\mathbf{V}, \Psi) \tag{55}$$

and the fact that $\{\mathcal{U}, \mathcal{V}\}$ is canonical gives

$$\mathbf{E} = -\mathcal{W}(\mathcal{U}, \Psi)\mathcal{W}(\mathcal{V}, \Psi)^{-1}. \tag{56}$$

Substituting the definitions of the **K**, **S**, and **T** matrices gives

$$\begin{aligned}
\mathbf{K} &= -\mathcal{W}(\mathbf{F}, \Psi)\mathcal{W}(\mathbf{G}, \Psi)^{-1} & (57)\\
\mathbf{S} &= -\mathcal{W}(\mathbf{F} - i\mathbf{G}, \Psi)\mathcal{W}(\mathbf{F} + i\mathbf{G}, \Psi)^{-1} & (58)\\
\mathbf{T} &= -\mathcal{W}(\mathbf{F}, \Psi)\mathcal{W}(\mathbf{F} + i\mathbf{G}, \Psi)^{-1}. & (59)
\end{aligned}$$

For a set of wave functions given by

$$\Psi = \mathbf{F}\mathbf{A} + \mathbf{G}\mathbf{B} \tag{60}$$

this yields

$$\begin{aligned}
\mathbf{K} &= \mathbf{B}\mathbf{A}^{-1} & (61)\\
\mathbf{S} &= (\mathbf{A} - i\mathbf{B})(\mathbf{A} + i\mathbf{B})^{-1} & (62)\\
\mathbf{T} &= \mathbf{B}(i\mathbf{A} - \mathbf{B})^{-1} & (63)
\end{aligned}$$

We can use these expressions to write down the following relations:

$$\begin{aligned}
\mathbf{S} &= (\mathbf{I} - i\mathbf{K})(\mathbf{I} + i\mathbf{K})^{-1} & (64)\\
\mathbf{S} &= \mathbf{I} + 2\mathbf{T} & (65)\\
\mathbf{K} &= i(\mathbf{S} - \mathbf{I})(\mathbf{S} + \mathbf{I})^{-1} & (66)\\
\mathbf{K} &= i\mathbf{T}(\mathbf{I} + \mathbf{T})^{-1} & (67)\\
\mathbf{T} &= \mathbf{K}(i\mathbf{I} - \mathbf{K})^{-1} & (68)\\
& & (69)
\end{aligned}$$

6 Properties derived from Wronskian relations

Let $\{\mathbf{U}, \mathbf{V}\}$ be canonical. Then from

$$\mathbf{U}^T\mathbf{U}' - \mathbf{U}'^T\mathbf{U} = 0 \tag{70}$$

if follows that

$$\mathbf{U}^T\mathbf{U}' = \mathbf{U}'^T\mathbf{U} \tag{71}$$

which gives

$$(\mathbf{U}'^T\mathbf{U})^T = \mathbf{U}'^T\mathbf{U} \tag{72}$$

and

$$(\mathbf{U}'\mathbf{U}^{-1})^T = \mathbf{U}'\mathbf{U}^{-1} \tag{73}$$

These relations also hold for $\mathbf{V}$.

Multiplying

$$\mathbf{U}^T\mathbf{V}' - \mathbf{U}'^T\mathbf{V} = c_E\mathbf{I} \tag{74}$$

from the right with $\mathbf{V}^{-1}$ and from the left with with $\mathbf{U}^{-T}$, taking the transpose and using the above symmetry relations gives

$$\mathbf{V}'\mathbf{V}^{-1} = \mathbf{U}'\mathbf{U}^{-1} + c_E\mathbf{V}^{-T}\mathbf{U}^{-1} \tag{75}$$

Multiplying Eq. (74) from the right with $\mathbf{V}^{-1}\mathbf{U}$ gives

$$\mathbf{U}^T\mathbf{V}'\mathbf{V}^{-1}\mathbf{U} - \mathbf{U}'^T\mathbf{U} = c_E\mathbf{V}^{-1}\mathbf{U} \tag{76}$$

which shows that

$$(\mathbf{V}^{-1}\mathbf{U})^T = \mathbf{V}^{-1}\mathbf{U} \tag{77}$$

7 The log-derivative matrix

Let

$$\Psi = \mathbf{U} + \mathbf{V}\mathbf{E} \tag{78}$$

then

$$\Psi' \equiv \mathbf{Y}\Psi \tag{79}$$

i.e.

$$\mathbf{U}' + \mathbf{V}'\mathbf{E} = \mathbf{Y}(\mathbf{U} + \mathbf{V}\mathbf{E}). \tag{80}$$

This equation can be solved for $\mathbf{E}$:

$$\mathbf{E} = -(\mathbf{V}' - \mathbf{Y}\mathbf{V})^{-1}(\mathbf{U}' - \mathbf{Y}\mathbf{U}) \tag{81}$$

To show that a symmetric $\mathbf{Y}$ matrix leads to a symmetric $\mathbf{E}$ matrix we can rewrite this equation as follows:

$$\mathbf{E} = -\mathbf{V}^{-1}(\mathbf{V}'\mathbf{V}^{-1} - \mathbf{Y})^{-1}(\mathbf{U}'\mathbf{U}^{-1} - \mathbf{Y})\mathbf{U}. \tag{82}$$

Substituting Eq. (75) gives

$$\begin{aligned}
\mathbf{E} &= -\mathbf{V}^{-1}(\mathbf{V}'\mathbf{V}^{-1} - \mathbf{Y})^{-1}(\mathbf{V}'\mathbf{V}^{-1} - \mathbf{Y} - c_E\mathbf{V}^{-T}\mathbf{U}^{-1})\mathbf{U} && (83)\\
&= -\mathbf{V}^{-1}[\mathbf{I} - c_E(\mathbf{V}'\mathbf{V}^{-1} - \mathbf{Y})^{-1}\mathbf{V}^{-T}\mathbf{U}^{-1}]\mathbf{U} && (84)\\
&= -\mathbf{V}^{-1}\mathbf{U} - c_E\mathbf{V}^{-1}(\mathbf{Y} - \mathbf{V}'\mathbf{V}^{-1})^{-1}\mathbf{V}^{-T} && (85)
\end{aligned}$$

In particular, with

$$\mathbf{0} \equiv \mathbf{G} + i\mathbf{F} \tag{86}$$

we have

$$\begin{aligned}
\mathbf{K} &= -\mathbf{G}^{-1}\mathbf{F} - \mathbf{G}^{-1}(\mathbf{Y} - \mathbf{G}'\mathbf{G}^{-1})^{-1}\mathbf{G}^{-T} && (87)\\
\mathbf{S} &= \mathbf{0}^{-1}\mathbf{0}^* - 2i\mathbf{0}^{-1}(\mathbf{Y} - \mathbf{0}'\mathbf{0}^{-1})^{-1}\mathbf{0}^{-T} && (88)\\
\mathbf{T} &= -\mathbf{0}^{-1}\mathbf{F} - \mathbf{0}^{-1}(\mathbf{Y} - \mathbf{0}'\mathbf{0}^{-1})^{-1}\mathbf{0}^{-T} && (89)
\end{aligned}$$

8 Properties of K, S, T, and Ymatrices

Let

$$\Psi = \mathcal{U} + \mathcal{V}\mathbf{E} + \Gamma \tag{90}$$

where $\{\mathcal{U}, \mathcal{V}\}$ is a canonical set and

$$\mathcal{W}(\mathcal{U}, \Gamma) = \mathcal{W}(\mathcal{V}, \Gamma) = \mathbf{0} \tag{91}$$

Assume that Ψ is a solution of Schrödinger equation

$$[\hat{H} - E]\Psi = 0. \tag{92}$$

Since

$$\langle\langle\Psi|\hat{H} - E|\Psi\rangle\rangle - \langle\langle\Psi|\hat{H} - E|\Psi\rangle\rangle^T = -\frac{\hbar^2}{2}\mathcal{W}(\Psi, \Psi) \tag{93}$$

we have

$$\mathcal{W}(\Psi, \Psi) = 0 \tag{94}$$

Using the fact that $\{\mathcal{U}, \mathcal{V}\}$ is canonical and the Wronskians involving Γ are zero this gives

$$\mathbf{E} = \mathbf{E}^T. \tag{95}$$

Thus, the **K**, **S**, and **T**matrices are symmetric. Also, since

$$\mathbf{Y} = \Psi'\Psi^{-1} \tag{96}$$

it follows that the log-derivative matrix must be symmetric.

If, in addition, we assume the potential to be real, we can also use

$$[\hat{H} - E]\Psi^* = 0 \tag{97}$$

and consequently

$$\mathcal{W}(\Psi^*, \Psi) = 0. \tag{98}$$

Applying this relation to **K** matrix boundary conditions gives

$$\mathbf{K} - \mathbf{K}^\dagger = 0 \tag{99}$$

thus, since the **K** matrix is symmetric, it must also be real.

For **S** matrix boundary conditions we find

$$\mathbf{S}^\dagger\mathbf{S} = \mathbf{I} \tag{100}$$

and for **T** matrix boundary conditions we find

$$2\mathbf{T}^\dagger\mathbf{T} + \mathbf{T}^\dagger + \mathbf{T} = 0 \tag{101}$$

which can be rewritten to

$$(\mathbf{I} + 2\mathbf{T})^\dagger(\mathbf{I} + 2\mathbf{T}) = \mathbf{I}. \tag{102}$$

This last result agrees with the relation between the **T** and **S** matrices that was found earlier.

9 Canonical transformations

The real matrices $\mathbf{C}$ and $\mathbf{D}$ define a canonical transformation of the set $\{\mathcal{F},\mathcal{G}\}$ by

$$\overline{\mathcal{F}} = \mathcal{F}\mathbf{C} + \mathcal{G}\mathbf{D} \tag{103}$$
$$\overline{\mathcal{G}} = -\mathcal{F}\mathbf{D} + \mathcal{G}\mathbf{C} \tag{104}$$

if

$$\mathbf{C}^T\mathbf{C} + \mathbf{D}^T\mathbf{D} = \mathbf{I} \tag{105}$$
$$\mathbf{C}^T\mathbf{D} - \mathbf{D}^T\mathbf{C} = \mathbf{0} \tag{106}$$

These conditions are equivalent to the condition that $\mathbf{C} + i\mathbf{D}$ is unitary, i.e.,

$$(\mathbf{C} + i\mathbf{D})^\dagger(\mathbf{C} + i\mathbf{D}) = \mathbf{I} \tag{107}$$

which is equivalent to the condition that the real matrix

$$\left[\begin{array}{cc} \mathbf{C} & -\mathbf{D} \\ \mathbf{D} & \mathbf{C} \end{array}\right] \tag{108}$$

is orthonormal. Note that

$$(\mathbf{C} + i\mathbf{D})^{-1} = \mathbf{C}^T - i\mathbf{D}^T \tag{109}$$

If $\{\mathcal{F},\mathcal{G}\}$ is canonical it follows that $\{\overline{\mathcal{F}},\overline{\mathcal{G}}\}$ is canonical and that

$$\mathcal{W}(\overline{\mathcal{F}},\overline{\mathcal{G}}) = \mathcal{W}(\mathcal{F},\mathcal{G}). \tag{110}$$

In supermatrix notation the transformation is given by

$$[\overline{\mathcal{F}}\ \overline{\mathcal{G}}] = [\mathcal{F}\ \mathcal{G}]\left[\begin{array}{cc} \mathbf{C} & -\mathbf{D} \\ \mathbf{D} & \mathbf{C} \end{array}\right]. \tag{111}$$

and the inverse is

$$[\mathcal{F}\ \mathcal{G}] = [\overline{\mathcal{F}}\ \overline{\mathcal{G}}]\left[\begin{array}{cc} \mathbf{C}^T & \mathbf{D}^T \\ -\mathbf{D}^T & \mathbf{C}^T \end{array}\right]. \tag{112}$$

A canonical transformation of $\{\mathcal{F},\mathcal{G}\}$ induces a transformation in $\mathbf{A}$ and $\mathbf{B}$ via the definition

$$\Psi = \mathcal{F}\mathbf{A} + \mathcal{G}\mathbf{B} \equiv \overline{\mathcal{F}}\,\overline{\mathbf{A}} + \overline{\mathcal{G}}\,\overline{\mathbf{B}} \tag{113}$$

Thus we find

$$\overline{\mathbf{A}} = \mathbf{C}^T\mathbf{A} + \mathbf{D}^T\mathbf{B} \tag{114}$$
$$\overline{\mathbf{B}} = -\mathbf{D}^T\mathbf{A} + \mathbf{C}^T\mathbf{B} \tag{115}$$

and its inverse

$$\mathbf{A} = \mathbf{C}\overline{\mathbf{A}} - \mathbf{D}\overline{\mathbf{B}} \tag{116}$$
$$\mathbf{B} = \mathbf{D}\overline{\mathbf{A}} + \mathbf{C}\overline{\mathbf{B}} \tag{117}$$

If we substitute these expressions into Eqs. (61) and use the unitarity of the matrices $\mathbf{C} \pm i\mathbf{D}$ we can derive

$$\mathbf{K} = (\mathbf{D} + \mathbf{C}\overline{\mathbf{K}})(\mathbf{C} - \mathbf{D}\overline{\mathbf{K}})^{-1} \tag{118}$$
$$\mathbf{S} = (\mathbf{C} - i\mathbf{D})\overline{\mathbf{S}}(\mathbf{C}^T - i\mathbf{D}^T) \tag{119}$$

and the inverse relations

$$\overline{\mathbf{K}} = (-\mathbf{D}^T + \mathbf{C}^T\mathbf{K})(\mathbf{C}^T + \mathbf{D}^T\mathbf{K})^{-1} \tag{120}$$
$$\overline{\mathbf{S}} = (\mathbf{C}^T + i\mathbf{D}^T)\mathbf{S}(\mathbf{C} + i\mathbf{D}) \tag{121}$$

10 Construction of canonical transformations

We will look for a canonical transformation that gives $\overline{\mathbf{K}} = \mathbf{0}$ or, equivalently $\overline{\mathbf{S}} = \mathbf{I}$. The transformation will not be unique, since if $\{\mathbf{C}, \mathbf{D}\}$ satisfies these conditions, the transformation $\{\mathbf{C}', \mathbf{D}'\}$ with

$$\mathbf{C}' = \mathbf{C}\mathbf{Q} \tag{122}$$
$$\mathbf{D}' = \mathbf{D}\mathbf{Q}, \tag{123}$$

where $\mathbf{Q}$ is orthogonal, is also canonical and satisfies the same conditions. The condition $\overline{\mathbf{S}} = \mathbf{I}$ gives

$$\mathbf{S} = (\mathbf{C}_1 - i\mathbf{D}_1)(\mathbf{C}_1^T - i\mathbf{D}_1^T) \tag{124}$$

Below we will show that $\mathbf{S}$, which is symmetric and unitary, has a symmetric unitary square root, thus we can take

$$\mathbf{C} = \mathrm{Re}(\mathbf{S}^{\frac{1}{2}}) \tag{125}$$
$$\mathbf{D} = -\mathrm{Im}(\mathbf{S}^{\frac{1}{2}}). \tag{126}$$

To prove that this symmetric square root exists we use the following theorem

Theorem 1 *A complex symmetric unitary matrix* $\mathbf{S}$ *has a spectral decomposition*

$$\mathbf{S} = \mathbf{Q}\Lambda\mathbf{Q}^T \tag{127}$$

where $\mathbf{Q}$ *is real and orthogonal and* Λ *is diagonal*

Proof: let

$$\mathbf{S} = \mathbf{S}_r + i\mathbf{S}_i \tag{128}$$

where $\mathbf{S}_r$ and $\mathbf{S}_i$ are real and symmetric. From the unitarity of $\mathbf{S}$ it follows that $\mathbf{S}_r$ and $\mathbf{S}_i$ commute, thus they must have a common set of eigenvectors $\mathbf{Q}$,

$$\mathbf{S}_r\mathbf{Q} = \mathbf{Q}\Lambda_r \tag{129}$$
$$\mathbf{S}_i\mathbf{Q} = \mathbf{Q}\Lambda_i. \tag{130}$$

From this it follows that

$$\mathbf{S} = \mathbf{Q}(\Lambda_r + i\Lambda_i)\mathbf{Q}^T \tag{131}$$

q.e.d.

To avoid the use of complex matrices we can can start with the eigenvalue decomposition of the $\mathbf{K}$ matrix, i.e.,

$$\mathbf{K} = \mathbf{Q}\Lambda\mathbf{Q}^T \tag{132}$$

and substitute this into the relation between the $\mathbf{S}$ and $\mathbf{K}$ matrices

$$\mathbf{S} = (\mathbf{I} - i\mathbf{K})(\mathbf{I} + i\mathbf{K})^{-1} \tag{133}$$
$$= \mathbf{Q}(\mathbf{I} - i\Lambda)\mathbf{Q}^T[\mathbf{Q}(\mathbf{I} + i\Lambda)\mathbf{Q}^T]^{-1} \tag{134}$$
$$= \mathbf{Q}(\mathbf{I} - i\Lambda)(\mathbf{I} + i\Lambda)^{-1}\mathbf{Q}^T \tag{135}$$
$$= \mathbf{Q}(\mathbf{I} - i\Lambda)^2(\mathbf{I} + \Lambda^2)^{-1}\mathbf{Q}^T. \tag{136}$$

We can now compute the square root analytically and we find

$$\mathbf{C} = \mathbf{Q}(\mathbf{I} + \Lambda^2)^{-\frac{1}{2}}\mathbf{Q}^T \tag{137}$$
$$\mathbf{D} = \mathbf{Q}(\mathbf{I} + \Lambda^2)^{-\frac{1}{2}}\Lambda\mathbf{Q}^T. \tag{138}$$

Since canonical transformations are determined up to an arbitrary orthonormal multiplication from the right we can also use

$$\mathbf{C} = \mathbf{Q}(\mathbf{I} + \Lambda^2)^{-\frac{1}{2}} \tag{139}$$
$$\mathbf{D} = \mathbf{Q}(\mathbf{I} + \Lambda^2)^{-\frac{1}{2}}\Lambda. \tag{140}$$

One may substitute these expressions into Eq. (120) to verify that $\overline{\mathbf{K}} = 0$.