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Phase Equivalent Potentials in Reaction Matrix Theory

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Abstract

The general class of phase equivalent nonlocal potentials is examined using standard reaction matrix methods. The relationship between phase equivalent overlap matrices is derived and it is found that the matrices fall into four general classes.

It was first shown by Bargmann (1949) that a potential which results in a given phase shift is actually a member of a whole class of phase equivalent potentials. Cook (1972) used a reaction matrix technique to illustrate this lack of uniqueness by calculating the potential in terms of Wigner and Eisenbud (1947) reaction matrix parameters, but did not determine what the general class of potentials should be.

In this paper, we determine the most general form for the overlap matrix **B** which results in a given set of phase shifts. A transformation of any orthogonal matrix to give four matrices, each phase equivalent to **B**, is found. The construction of all possible phase equivalent matrices is a trivial extension.

Review of Theory

The radial wavefunction ψ_l of a particle of mass M scattered by a target obeys the relation

$$\frac{\mathrm{d}^2\psi_l(r)}{\mathrm{d}r^2}+\left(\frac{2M(E-V)}{\hbar^2}-\frac{l(l+1)}{Mr^2}\right)\psi_l(r)=0\,, \tag{1}$$

where E is the total energy of the particle, V the interaction potential operator and l the orbital angular momentum. A cutoff radius $r = a$ is chosen at which $V\psi_l = 0$, and a function R_l is defined by

$$\psi_l(a)=R_l\,a\big(\mathrm{d}\psi_l/\mathrm{d}r\big)_{r=a}\,. \tag{2}$$

Equation (1) is then solved across the interior region $0 < r < a$ with the boundary conditions

$$\big(\mathrm{d}U_\lambda/\mathrm{d}r\big)_{r=a}=(b/a)U_\lambda(a)\,, \tag{3}$$

and the $U_\lambda(r)$ form an orthonormal set on the above interval for each partial wave.

Dropping the l suffix, we find

$$\psi(r) = \sum_\lambda A_\lambda(E)\, U_\lambda(r), \qquad V\psi = \sum_\lambda A_\lambda(E)\, V_\lambda(r)\, U_\lambda(r), \tag{4}$$

where

$$A_\lambda(E) = \frac{1}{2M}\frac{U_\lambda(a)}{E_\lambda - E}\left(\frac{\mathrm{d}\psi}{\mathrm{d}r}\right)_{r=a}\left(1 - b\mathscr{R}\right), \qquad \mathscr{R} = \frac{R}{1-bR}, \tag{5}$$

and the Wigner–Eisenbud reaction matrix R, with the notation $U_\lambda^2(a)/2Ma = \gamma_\lambda^2$ is given by

$$R = \frac{1}{2Ma}\sum_\lambda \frac{U_\lambda^2(a)}{E_\lambda - E} = \sum_\lambda \frac{\gamma_\lambda^2}{E_\lambda - E}, \tag{6}$$

the set $\{E_\lambda\}$ of energy eigenvalues following from the boundary conditions (3).

Let $W_\mu(r)$ be the solutions to equations (1) and (3) when $V = 0$. There exist the expansions

$$\text{(i)}\quad U_\lambda(r) = \sum_\mu B_{\lambda\mu}\, W_\mu(r), \qquad \text{(ii)}\quad V_\lambda\, U_\lambda(r) = \sum_\mu V_{\lambda\mu}\, W_\mu(r), \tag{7}$$

where

$$\mathbf{B}\mathbf{B}^{\mathrm{T}} = \mathbf{I}, \tag{8}$$

that is, $\mathbf{B}$ is an orthogonal matrix, and

$$V_{\mu\lambda} = (E_\lambda - \varepsilon_\mu) B_{\lambda\mu}, \tag{9}$$

the ε_μ being the energy eigenvalues obtained with $V = 0$.

From equations (7) we have

$$U_\lambda(a) = \sum_\mu B_{\lambda\mu}\, W_\mu(a), \tag{10}$$

where $U_\lambda(a)$ and $W_\mu(a)$ are known quantities, thus giving constraints on $\mathbf{B}$. These constraints, together with the condition (8) leave $\frac{1}{2}(n^2 - 3n) + 1$ degrees of freedom for the elements of $\mathbf{B}$, where $\mathbf{B}$ is taken to be an $n \times n$ matrix. It is the arbitrariness of these degrees of freedom which defines phase equivalent potentials, since the reaction matrix (6) defines the phase shift as a function of E. It should be noted that because $\mathbf{B}$ is orthogonal there is a constraint on the terms of $U_\lambda(a)$ so that equation (10) removes $n-1$ rather than n degrees of freedom. It is significant that the number of degrees of freedom for an orthogonal matrix of one fewer dimensions, i.e. an $(n-1)\times(n-1)$ orthogonal matrix, is

$$\tfrac{1}{2}(n-1)(n-2) = \tfrac{1}{2}n^2 - \tfrac{3}{2}n + 1\,.$$

Equivalent Overlap Matrices

We now use the notation

$$U_\lambda(a) \equiv |u\rangle, \qquad W_\mu(a) \equiv |w\rangle, \tag{11}$$

giving (from equation 10)

$$|u\rangle = \mathbf{B}|w\rangle\,. \tag{12}$$

It is always possible to find a vector $|b\rangle$ such that

$$|u\rangle = \alpha|w\rangle + \beta|b\rangle, \tag{13}$$

where

$$\langle w|b\rangle = 0, \qquad \langle u|u\rangle = \langle w|w\rangle = \langle b|b\rangle = 1, \tag{14}$$

so that

$$\alpha = \langle w|u\rangle, \qquad \beta|b\rangle = |u\rangle - \alpha|w\rangle, \qquad \alpha^2+\beta^2 = 1. \tag{15}$$

Let

$$\mathbf{B} = (\alpha|w\rangle + \beta|b\rangle)\langle w| \pm (\beta|w\rangle - \alpha|b\rangle)\langle b|\mathbf{DP} + (\mathbf{I} - |b\rangle\langle b|)\mathbf{PDP}, \tag{16}$$

in which $\mathbf{P}$ is a projection operator:

$$\text{(i)}\quad \mathbf{P} = \mathbf{I} - |w\rangle\langle w|, \qquad \text{(ii)}\quad \mathbf{P}^2 = \mathbf{P}. \tag{17}$$

Equations (16) and (13) satisfy (12). The matrix $\mathbf{D}$ in equation (16) is any orthogonal matrix in the space obtained by the projection excluding $|w\rangle$, that is,

$$\mathbf{PDPD}^{\mathrm{T}}\mathbf{P} = \mathbf{PD}^{\mathrm{T}}\mathbf{PDP} = \mathbf{P}. \tag{18}$$

The orthogonality condition (8) applies to equation (16) and may be verified by direct substitution, making use of the surrounding conditions.

Let $\mathbf{G}$ be an arbitrary orthogonal matrix satisfying

$$\mathbf{G}^{\mathrm{T}}\mathbf{G} = \mathbf{GG}^{\mathrm{T}} = \mathbf{I}. \tag{19}$$

To construct a matrix $\mathbf{D}$ obeying equation (18) we first try

$$\mathbf{D} = \mathbf{PGP} - \nu\mathbf{PG}|w\rangle\langle w|\mathbf{GP}, \tag{20}$$

in which case it is necessary that

$$(1-\nu g)^2 = \nu^2, \qquad \text{where} \qquad \langle w|\mathbf{G}|w\rangle = g.$$

The solution is $\nu = (g \pm 1)/(g^2-1)$, that is,

$$\nu = -(1-g)^{-1} \qquad \text{or} \qquad \nu = (1+g)^{-1}. \tag{21}$$

Starting from a particular orthogonal matrix $\mathbf{G}$, we find that the two choices of ν in equations (21) and the choice of sign in equation (16) usually lead to four distinct phase equivalent $\mathbf{B}$ matrices. If the matrix $\mathbf{G}$ is already phase equivalent to $\mathbf{B}$, the four matrices reduce to two, one of which is $\mathbf{G}$. For every matrix $\mathbf{B}'$ that is phase equivalent to any one of the four $\mathbf{B}$ matrices, there are two distinct matrices $\mathbf{D}$ that are orthogonal in the space truncated by the removal of $|w\rangle$. All possible phase equivalent matrices $\mathbf{B}'$ can therefore be generated using as a starting point the set of *all* possible orthogonal matrices $\mathbf{D}$ in the truncated space. All such $\mathbf{B}'$ matrices then obey equation (10) and are orthogonal in the full space, therefore leading to the same set of phase shifts as obtained from $\mathbf{B}$. As discussed in the preceding section, the number of degrees of freedom is exactly right.

It is interesting to note that if equation (10) holds in an n-dimensional channel space such that

$$U_{\lambda c}(a) = \sum_{\mu} B_{\lambda\mu} W_{\mu c}(a) \tag{22}$$

then, if we choose the same $\mathbf{B}$ matrix for all channels, it is fully defined by equation (22) and there are no phase equivalent overlap matrices.

In conclusion, we have thus defined here a general class of overlap matrices which lead to a class of phase equivalent local or nonlocal potentials. We intend to investigate this class numerically to find out more about the possible general structure of **B**.

References

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