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Use of the K Matrix in Nuclear Reaction Theories*

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In the original article the formal solution to the integral equation for the reactance operator K was found and shown to differ from the generally accepted form. The incorrect expression for K has been used in projection-operator formalisms for nuclear reactions by Bloch and Gillet (BG) and by MacDonald and Mekjian (MM). We applied these scattering formalisms to a simple soluble model. The discrepancy arising from the use of the incorrect K was found to have no observable consequences for the MM treatment. We did not succeed in finding an explicit expression for the discrepancy between the BG prediction and the exact result for the simple scattering model. In this addendum the discrepancy of the BG formalism for the simple scattering model is found. This discrepancy is found to be nonzero at all energies. In the neighborhood of certain energies for zero-range potential scattering, the BG discrepancy can become very large. In addition, by examining the explicit expressions for the K matrix for zero-range potential scattering, we are able to provide a simple interpretation of the difference between the correct form of the reactance operator and the generally accepted incorrect form.

IN the paper for which this addendum is written,[1] the formal solution to the integral equation for the reactance operator K was found and shown to differ from the generally accepted form. The incorrect expression for K had been used in projection-operator formalisms for nuclear reactions by Bloch and Gillet (BG) and by MacDonald and Mekjian (MM). In our paper we applied these formalisms to a simple soluble scattering model and sought to determine what discrepancy with the correct result was caused by the use of the incorrect expression for K. The discrepancy that occurred in the MM treatment was identified and found to have no observable effect. However, we did not succeed in finding an explicit expression for the BG discrepancy.

In this addendum we derive the explicit expression for the BG discrepancy. It is found to be nonzero at all energies, and under certain circumstances the discrepancy can become very large. In addition, by examining the explicit expressions for the K matrix for zero-range potential scattering, we are able to provide a simple interpretation of the difference between the correct form of the reactance operator and the generally accepted incorrect form.

The material presented below constitutes an addition to Sec. IV of the original paper, in which the discussion of the BG and MM discrepancies for seperable s-wave potential scattering is carried to completion. This is followed by Sec. V, in which the case of zero-range potential scattering is used to provide an explicit realization of some of our formal results.

If we make use of Eq. (19), the relationships among $\hat{\Gamma}$, $\hat{\Delta}$, Γ_0, and Δ_0 can be expressed by

$$\hat{\Gamma}=\Gamma_0+\Gamma_0Q\hat{K}\hat{\Gamma}-\pi^2\Delta_0Q\hat{K}\hat{\Delta}, \tag{70a}$$

$$\hat{\Delta}=\Delta_0+\Gamma_0Q\hat{K}\hat{\Delta}+\Delta_0QK\hat{\Gamma}. \tag{70b}$$

Substitution of these expressions into Eqs. (61) and use of Eqs. (54) and (56) leads to the following results:

$$y=x+(xy-vz)(1-w)^{-1}, \tag{71a}$$

$$z=v+(xy-vy)(1-w)^{-1}, \tag{71b}$$

where

$$v=v(E)=\pi\langle\gamma\mid\Delta_0(E)Q\mid\gamma\rangle. \tag{61e}$$

Equations (71) maybe solved for y and z, with the result

$$z=v(1-w)^2/[v^2+(1-w-x)^2], \tag{72a}$$

$$y=(1-w)[x(1-w-x)-v^2]/[v^2+(1-w-x)^2]. \tag{72b}$$

The results of Eqs. (72) can then be substituted into Eq. (62) to give

$$k_1=(1-w)(1-w-x)/[(1-w-x)^2+v^2], \tag{73a}$$

$$k_2=v^2(1-w)/\{(1-w-x)[(1-w-x)^2+v^2]\}. \tag{73b}$$

One can readily verify that $k_1+k_2=k$.

Thus, we can corroborate the existence of the discrepancy k_2 without making use of explicit expressions for the projection operators P and Q.

In the MM treatment, the quantity v is given by

$$v_{MM}=\epsilon\langle 0\mid V_0\mid 0\rangle/[(E-W_0)^2+\epsilon^2], \tag{74a}$$

whereas in the BG treatment it is given by

$$v_{BG}=\epsilon\int dW\ \langle W\mid V_0\mid W\rangle/[(E-W)^2+\epsilon^2] \underset{\epsilon\to 0}{\longrightarrow}\pi\langle E\mid V_0\mid E\rangle. \tag{74b}$$

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[1] W. Tobocman and M. A. Nagarjan, Phys. Rev. **163**, 1011 (1967).

In the limit $\epsilon\to 0$ it is seen that v_{MM} vanishes except when $E=W_0$. Thus, the discrepancy k_2 vanishes for all energies except $E=W_0$. On the other hand, v_{BG} does not vanish. Hence the discrepancy k_2 does not vanish for the BG treatment. In Sec. V we will apply the formalism to the zero-range potential model and determine the importance of k_2 for that model.

V. APPLICATION TO ZERO-RANGE POTENTIAL SCATTERING

To illustrate in more detail the results presented above, we will consider a particular case of scattering by a separable potential, namely, scattering by a zero-range potential. Let the Hamiltonian of the system be

$$H=-d^2/dr^2-[(1/r)+b]\delta(r), \tag{75a}$$

$$0\leq r\leq\infty, \tag{75b}$$

where it is understood that

$$\delta(r)=\lim_{\eta\to 0}\delta(r-\eta). \tag{76}$$

Let the unperturbed Hamiltonian be

$$H_0=-(d^2/dr^2)-[(1/r)+b_0]\delta(r), \tag{77}$$

so that the perturbation is

$$\begin{aligned}V&=H-H_0=(b_0-b)\,\delta(r)\\&=|\,\delta(r)\,(b_0-b)^{1/2}\rangle\langle\delta(r)\,(b_0-b)^{1/2}\,|\\&=|\,\gamma\rangle\langle\gamma\,|.\end{aligned} \tag{78}$$

The wave function for the unperturbed state is

$$\Psi_\kappa(r)=\sin(\kappa r+\delta_0), \tag{79a}$$

$$\delta_0=-\tan^{-1}(\kappa/b_0), \tag{79b}$$

$$H\Psi_\kappa(r)=\kappa^2\Psi_\kappa(r). \tag{79c}$$

The scattering function (collision matrix) is then

$$\mathfrak{U}=\exp(i2\delta)=(b-i\kappa)/(b+i\kappa) \tag{80a}$$

$$=\exp(i2\delta_0)\,(1-2i\mathfrak{I}) \tag{80b}$$

$$=\exp(i2\delta_0)\,(1-i\mathfrak{K})/(1+i\mathfrak{K}), \tag{80c}$$

where the transition amplitude (T matrix) is

$$\mathfrak{I}=\kappa^{-1}\langle\Psi_\kappa\,|\,T\,|\,\Psi_\kappa\rangle \tag{81a}$$

and the reaction amplitude (K matrix) is

$$\mathfrak{K}=\kappa^{-1}\langle\Psi_\kappa\,|\,K\,|\,\Psi_\kappa\rangle. \tag{81b}$$

For our simple model these quantities can be evaluated explicitly to reveal their relationships.

Since the perturbation is separable, the amplitudes defined above can be calculated from Eqs. (9) and (10) in the following manner:

$$\begin{aligned}\mathfrak{I}&=\kappa^{-1}\langle\Psi_\kappa\,|\,V+VGV\,|\,\Psi_\kappa\rangle\\&=\kappa^{-1}(b_0-b)\,\sin^2\delta_0\,(1+\langle\gamma\,|\,G\,|\,\gamma\rangle),\end{aligned} \tag{82a}$$

$$\begin{aligned}\mathfrak{K}&=\kappa^{-1}\langle\Psi_\kappa\,|\,V+V\bar{\Gamma}V\,|\,\Psi_\kappa\rangle\\&=\kappa^{-1}(b_0-b)\,\sin^2\delta_0\,(1+\langle\gamma\,|\,\bar{\Gamma}\,|\,\gamma\rangle).\end{aligned} \tag{82b}$$

The scattering Green's function G for this system has a simple form which we can use to evaluate

$$\begin{aligned}\langle\gamma\,|\,G\,|\,\gamma\rangle&=\langle\gamma\,|\,-\kappa^{-1}\sin(\kappa r_<+\delta)\,\exp i(\kappa r_>+\delta)\,|\,\gamma\rangle\\&=(b-b_0)\,\kappa^{-1}\sin\delta\,\exp i\delta.\end{aligned} \tag{83}$$

Substituting this back into Eq. (82a) and using the fact that

$$\begin{aligned}(b_0-\kappa)\,\kappa^{-1}&=(\cot\delta-\cot\delta_0)\\&=\sin(\delta_0-\delta)/\sin\delta\,\sin\delta_0,\end{aligned} \tag{84}$$

we find

$$\begin{aligned}\mathfrak{I}&=-\exp[-i(\delta-\delta_0)]\sin(\delta-\delta_0)\\&=\kappa(b_0-b)\,(b_0-i\kappa)^{-1}(b+i\kappa)^{-1}.\end{aligned} \tag{85}$$

To evaluate the expression for the reaction amplitude shown in Eq. (82b), one is tempted to use for $\bar{\Gamma}$ the principal-part Green's function Γ, where

$$\Gamma\Psi(r)=-\int_0^\infty dr'\,\kappa^{-1}\sin(\kappa r_<+\delta)\,\cos(\kappa r_>+\delta)\,\Psi(r'). \tag{86}$$

This would be the conventional, incorrect choice. By the definition given in Eq. (12), $\bar{\Gamma}$ is a solution of the integral equation

$$\bar{\Gamma}=\Gamma_0+\Gamma_0V\bar{\Gamma}, \tag{87a}$$

$$\Gamma_0\Psi(r)=-\int_0^\infty dr'\,\kappa^{-1}\sin(\kappa r_<+\delta_0)\,\cos(\kappa r_>+\delta_0)\,\Psi(r'). \tag{87b}$$

Both Γ and $\bar{\Gamma}$ are inverses of κ^2-H; but $\bar{\Gamma}$ is seen to be that inverse of κ^2-H which has the same asymptotic behavior as Γ_0. This information permits us to see that

$$\begin{aligned}\bar{\Gamma}\Psi(r)=-\int_0^\infty dr'\,[\kappa\cos(\delta-\delta_0)]^{-1}\sin(\kappa r_<+\delta)\\\times\cos(\kappa r_>+\delta_0)\,\Psi(r').\end{aligned} \tag{88}$$

The factor $[\cos(\delta-\delta_0)]^{-1}$ is required for normalization.

Proceeding now with the evaluation of the reaction amplitude, we note that

$$\langle\gamma\,|\,\bar{\Gamma}\,|\,\gamma\rangle=(b-b_0)[\kappa\cos(\delta-\delta_0)]^{-1}\sin\delta\,\cos\delta_0. \tag{89}$$

When this is substituted into Eq. (82b) and use is made of Eq. (84), we find

$$\begin{aligned}\mathfrak{K}&=-\tan(\delta-\delta_0)\\&=\kappa(b_0-b)\,(\kappa^2+b_0b)^{-1}.\end{aligned} \tag{90}$$

Next we will apply the BG projection-operator formalism to our zero-range potential scattering model. The first step is to identify the wave functions used in

the definitions of the projection operators displayed in Eq. (68)

$$\langle r \mid 0\rangle = \langle r \mid -b_0^2\rangle = (2b_0)^{1/2}\exp(-b_0 r), \quad (91a)$$

$$\langle r \mid W\rangle = \langle r \mid \kappa^2\rangle = (\pi\kappa)^{-1/2}\sin(\kappa r+\delta_0). \quad (91b)$$

Using these expressions in Eqs. (61) and (68), we find

$$w = 2b_0(b_0-b)/(\kappa^2+b_0^2), \quad (92a)$$

$$x = -b_0(b_0-b)/(\kappa^2+b_0^2), \quad (92b)$$

$$v = -\kappa(b_0-b)/(\kappa^2+b_0^2). \quad (92c)$$

The reaction amplitude is

$$\begin{aligned}\mathcal{K} &= \mathcal{K}_1+\mathcal{K}_2 = \kappa^{-1}\langle\Psi_\kappa \mid \hat{K} \mid \Psi_\kappa\rangle(k_1+k_2)\\ &= [\langle\Psi_\kappa \mid V \mid \Psi_\kappa\rangle/\kappa(1-w)](k_1+k_2)\\ &= (b_0-b)\kappa(k_1+k_2)/(b_0^2+\kappa^2)(1-w). \quad (93)\end{aligned}$$

Combining Eqs. (73), (92), and (93) gives

$$\mathcal{K}_1 = AB/(A^2+B^2), \quad (94a)$$

$$\mathcal{K}_2 = A^3/B(A^2+B^2), \quad (94b)$$

$$A = \kappa(b_0-b) = \kappa^2(\cot\delta-\cot\delta_0), \quad (94c)$$

$$B = \kappa^2+b_0 b = \kappa^2(1+\cot\delta\cot\delta_0). \quad (94d)$$

We know that $\mathcal{K} = \mathcal{K}_1+\mathcal{K}_2 = \tan(\delta_0-\delta)$. The question is how great an error results from neglecting $\mathcal{K}_2$. It is clear that

$$\mathcal{K}_2/\mathcal{K} = A^2/(A^2+B^2) \quad (95)$$

will be small when $b_0-b \ll \kappa$ or when $\kappa^2 \ll b_0 b$. On the other hand, when b is chosen to have the opposite sign to b_0, then B will vanish at the energy $\kappa^2 = -b_0 b$. Clearly, in the neighborhood of this energy $\mathcal{K}_2$ will be large and $\mathcal{K}_1$ will be small, and the neglect of $\mathcal{K}_2$ will lead to poor results.

Erratum

Fission Energetics and Neutron Emission in 13-MeV Proton-Induced Fission of ^{226}Ra, E. KONECNY AND H. W. SCHMITT [Phys. Rev. **172**, 1213 (1968)]. In Table I, line 6, the entry under "Experimental" should read $\partial\nu/\partial m^* = 0.077$ n/amu rather than 0.77 n/amu.