Discrete-basis formalism for reaction theory

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1. Motivation

There are two good reasons to formulate reaction theory in a discrete basis. First, it allows Hamiltonian models to be applied in a very controlled way in a configuration-interaction formulations, as in the multi-configuration shell model. In contrast, the formulation through generator coordinates is very difficult to relate back to the Hamiltonian expressed in the nucleonic degrees of freedom [1]. The main application I have in mind is a model for neutron-induced fission based on nucleon-nucleon interactions and can deal with the complexity of the problem at finite excitation energy. The other reason for a discrete basis is that the numerical computation can be easily implemented by ordinary linear algebra operations, once the needed Hamiltonian matrice has been constructed.

The object here is to compute S-matrix elements in a regime where there are many internal levels, but without making statistical approximations on the S-matrix itself. The derivation differs from the usual ones in that S-matrix elements are calculated directly without going throught the eigenchannel representation.

2. Coupling a channel to a resonance

The simplest case is a single channel and a single resonant state coupled to it. The scattering wave function is represented by its amplitudes on a uniform spatial mesh. Here I will simplify the problem by assuming that the coupling between the resonance and scattering wave function is localized to the first mesh point. The Hamiltonian parameters in this formulation are: E_r and v_r, the diagonal energy of the resonance and its coupling matrix element to the mesh; t, the (negative) Hamiltonian matrix element between adjacent mesh points; and E, the energy of the system with respect to the middle of the band of scattering states. The Hamiltonian has the form

$$H = \begin{bmatrix} E_r & v_r & 0 & 0 & \\ v_r & 0 & t & 0 & \\ 0 & t & 0 & t & \\ 0 & 0 & t & 0 & \\ & & & & \ddots \end{bmatrix}, \tag{1}$$

governing the resonance amplitude ϕ_0 as the first entry and scattering wave function amplitudes $(\phi_1, \phi_2, ...)$ on mesh points thereafter. That part of the Hamiltonian is an approximation to the continuous coordinate representation with a mesh spacing of Δx taking the off-diagonal H as $t = -\hbar^2/2m(\Delta x)^2$.

Except for an overall phase, the scattering wave function at mesh point $n \geq 1$ is expressed in terms of t and E by

$$\phi_n = e^{-ikn} - re^{ikn} \tag{2}$$

where r is the reflection and amplitude and k is given by

$$k = \cos^{-1}(E/2t) \quad \text{or} \quad E = 2t\cos(k). \tag{3}$$

In the absence of any coupling to the resonance, ie. if $v_r = 0$, Eq. (2) is a scattering eigenstate with $r = 1$. It is a simple algebraic exercise to solve the Hamiltonian equation $H\phi = E\phi$ imposing Eq. (2) for amplitudes beyond the interaction point. The equations for the first two row are

$$\begin{aligned} (E_r - E)\phi_0 + v_r\phi_1 &= 0 \\ v_r\phi_0 - E\phi_1 + t\phi_2 &= 0 \end{aligned} \tag{4}$$

Substituting Eq. (2) for ϕ_1 and ϕ_2, the equations may be solved for the reflection amplitude r. The result is

$$\begin{aligned} r(E) &= \frac{1 - e^{-ik}v_r^2/t(E - E_r)}{1 - e^{ik}v_r^2/t(E - E_r)}. \\ &= \frac{E_r - E + e^{-ik}v_r^2/t}{E_r - E + e^{+ik}v_r^2/t} \end{aligned} \tag{5}$$

Note that t is assumed to be negative to define which are incoming and outgoing fluxes. The reflection amplitude has a pole at $E = E_0 + i\Gamma_r/2$ where the shifted resonant energy is $E_0 = E_r + \cos(k)v_r^2/t$ and

$$\Gamma_r = 2\sin(k)\frac{v_r^2}{|t|}. \tag{6}$$

is the resonance width. Note that we require $t < 0$ in defining Γ_r.

Exercise: show that $r(E) = e^{2ik}$ if $E_r = 0$ and $v_r = t$. In effect, a extra point has been added to the mesh and the free-particle wave function is shifted by $n \to n + 1$.

2b. Including a potential in the entrance channel

In conventional formulations of reaction theory, one starts with the solutions of the potential

scattering problem. Let us make the connection that formulation. It is easy to include a scattering potential V_n in the scattering channel as diagonal matrix elements $H_{nn} = V_n$ in the Hamiltonian. Solving the Hamiltonian for pure potential scattering, one finds the incoming and outgoing wave solutions I and O. We normalize these outside the scattering potential as

$$I_n \to e^{-ikn} e^{-i\delta}$$

$$O_n \to e^{ikn} e^{+i\delta}.$$

Here δ is the scattering phase shift for potential scattering. The potential scattering wave function with both incoming and outgoing components is

$$U = (I - O) = -2i\Im(I) = 2i\sin(kn + \delta). \tag{7}$$

We next solve Hamiltonian equation including the resonance. In the external region, the wave function ϕ can be expressed

$$\phi = I - rO \tag{8}$$

where as before r is the reflection amplitude. It satisfied the unitarity condition $|r| = 1$ which we will now show by explicit construction.

As in the previous section, we assume that the coupling takes place at a single mesh point p. First note that ϕ up to and including mesh point $n = p$ is proportional to U; we write it as

$$\phi_n = cU_n \;\; n \leq p. \tag{9}$$

The proportionality constant c may be determined by matching inner and outer wave functions at p:

$$c(I_p - O_p) = I_p - rO_p \tag{10}$$

Next we require that the ϕ solves the Hamiltonian equation at p:

$$t\phi_{p-1} + \left(V_p + \frac{v_r^2}{E - E_r} - E\right)\phi_p + t\phi_{p+1} = 0 \tag{11}$$

We also make use of the solution in the absence of the resonance,

$$tU_{p-1} + (V_n - E)\,U_p + tU_{p+1} = 0. \tag{12}$$

Combining these equation we may solve for r as

$$r = \frac{tW + I_p U_p v_r^2/(E - E_r)}{tW + O_p U_p v_r^2/(E - E_r)}. \tag{13}$$

Here

$$W = O_{p+1}I_p - I_{p+1}O_p = 2i\sin(k) \tag{14}$$

is the discretized wronskian of the outgoing and incoming wave. In Eq (13), W and U are purely imaginary, I_p is complex conjugate of O_p, and the rest of the variables are real. Thus the numerator and denominator have the same modulus. This proves that $|r| = 1$ as required by single-channel unitarity.

The width of the resonance can be extracted by finding the pole of r in the complex plane assuming that all quantities are fixed except the explicit E-dependence in the formula. The result is

$$\Gamma_r = |U_p|^2 \frac{v_r^2}{2t\sin(k)}. \tag{15}$$

Note that Eq. (6) can be recovered from this formula taking U from Eq. (2) with $r = 1$.

3. A single channel and many resonances

Eq. (5) is easily generalized to the situation where there are many internal resonances coupling to the channel. Consider a set internal states labelled by i with Hamiltonian matrix elements H_a within the space and $\vec{v}$ coupling the internal states to the scattering wave function on the first site. Then Eq. (5) becomes

$$r(E) = \frac{1 - e^{-ik}\sum_{i,j} v_i G_{ij} v_j/t}{1 - e^{ik}\sum_{i,j} v_i G_{ij} v_j/t} \tag{16}$$

where $G = (E - H)^{-1}$. This formula can be easily implemented in the discrete basis. It just requires few lines of coding and a call to a linear algebra library.

4. Two channels

First consider the case where there are two channels a and b coupled to a single resonance. Let us take a as the entrance channel so there is an outgoing wave in channel b. Then the amplitudes on the first and second mesh points in channel b satisfy

$$\phi_{b,2} = e^{ik_b}\phi_{b,1}. \tag{17}$$

Next write the Hamiltonian equation to be solved as an matrix equation for the amplitudes

ϕ_0, $\phi_{a,1}$, and $\phi_{b,1}$ putting the amplitudes for the second mesh points on the right-hand side:

$$\begin{bmatrix} E_r - E & v_a & v_b \\ v_a & -E & 0 \\ v_b & 0 & -E \end{bmatrix} \begin{pmatrix} \phi_0 \\ \phi_{a,2} \\ \phi_{b,1} \end{pmatrix} = \begin{pmatrix} 0 \\ -t_a\phi_{a,2} \\ -t_b\phi_{b,2} \end{pmatrix}. \tag{18}$$

The amplitude in the bottem entry of the vector on the righthand side can be moved into the Hamiltonian with the help of Eq. (17). The quantity $\phi_{a,2}$ in the middle entry of the vector can be divided out in the vectors on both sides of Eq. (18). The result is an ordinary inhomogeneous matrix equation for the amplitude ratios $(x_0, x_a, x_b) = (\phi_0, \phi_{a,1}, \phi_{b,1})/\phi_{a,2}$:

$$\begin{bmatrix} E_r - E & v_a & v_b \\ v_a & -E & 0 \\ v_b & 0 & -E + t_a e^{ik_a} \end{bmatrix} \begin{pmatrix} x_0 \\ x_a \\ x_b \end{pmatrix} = \begin{pmatrix} 0 \\ -t_a \\ 0 \end{pmatrix} \tag{19}$$

We solve the the equation for $\vec{x}$ and extract r from x_a using Eq. (8) and (13). $\phi_{a,2}$ is next determined from the expression $\phi_{a,2} = e^{-2ik_a} - re^{2ik_a}$, taking r from the last equation. Finlly, we multiply $\vec{x}$ by $\phi_{a,2}$ to get the rest of the wave function.

The modulus of the off-diagonal S-matrix element between the two channels can be computed from the particle current in the the channels. In particular, the current of particles from state i to state j is given by

$$j_{ij} = -iH_{ij}\left(\phi_i^*\phi_j - \phi_j^*\phi_i\right). \tag{20}$$

The current associated with the incoming wave function $e^{-ik_a n}$ is given by $2t_a \sin(k_a)$. The outgoing current in the same channel is $|r|^2$ times the incoming current. Finally, the current in channel b is

$$j_b = 2t_b \sin(k_b)|\phi_{b,1}|^2. \tag{21}$$

The square of the S-matrix elements coupling the entrance channel is just the ratio of outgoing currents to the incoming current. Thus,

$$|S_{aa}|^2 = |r|^2 \tag{22}$$

$$|S_{ab}|^2 = \frac{t_b \sin(k_b)}{t_a \sin(k_a)}|\phi_{b,1}|^2$$

The formalism can be simplified by making use of the formula to invert a matrix by blocks:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - Ca^{-1}B)^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix} \tag{23}$$

where A and D are square submatrices. This is applied to the matrix in Eq. (19) with

$$A = \begin{bmatrix} E_r - E & v_a \\ v_a & -E \end{bmatrix}$$

and $D = -E + t_b e^{ik_b}$. Then the matrix equation for the upper righthand block becomes

$$\begin{bmatrix} E_r - E - \frac{v_b^2}{-E+t_b e^{ik_b}} & v_a \\ v_a & -E \end{bmatrix} \begin{pmatrix} x_0 \\ x_a \end{pmatrix} = \begin{pmatrix} 0 \\ -t_a \end{pmatrix}. \tag{24}$$

After solving this equation for (x_0, x_a), we determine x_b from the lower left-hand block as

$$x_b = -\frac{1}{-E + t_b e^{ik_b}} x_0. \tag{25}$$

The S-matrix elements are then computed as before. The final formula for the reflection amplitude is

$$r(E) = \frac{E_r + \Delta_a + \Delta_b - i(\Gamma_b - \Gamma_a)/2 - E}{E_r + \Delta_a + \Delta_b - i(\Gamma_b + \Gamma_a)/2 - E} \tag{26}$$

where $\Delta_i = t_i \cos(k_i)$ and $\Gamma_i = 2|t_i| \sin(k_i)$.

The corresponding reflection coefficient $R = |r|^2$ is by

$$R = \frac{(E_r + \Delta_a + \Delta_b - E)^2 + (\Gamma_a - \Gamma_b)^2/4}{(E_r + \Delta_a + \Delta_b - E)^2 + (\Gamma_a + \Gamma_b)^2/4} \tag{27}$$

and the transmission coefficient T_{ab} from one channel to the other is

$$T_{ab} = 1 - R = \frac{\Gamma_a \Gamma_b}{(E_r + \sum_i \Delta_i - E)^2 + (\Gamma_a + \Gamma_b)^2/4} \tag{28}$$

Note that perfect transmission, ie. $T_{ab} = 1$, is only possible if the partial widths Γ_a and Γ_b are equal. The further requirement is that the energy is on resonance, $E = E_r + \sum_i \Delta_i$.

5. Generalization to multiple internal states and outgoing channels

The generalization to multiple internal states and outgoing channels is straightforward. With N_μ internal states and N_c outgoing channels, the matrix in Eq. (24) becomes an $(N_\mu + 1) \times (N_\mu + 1)$ matrix with a submatrix H_{int} for the internal Hamiltonian and a $1 \times (N_a + 1)$ matrix $\vec{v}_r$ for the coupling to the entrance channel. The coupling matrix elements to the outgoing channels becomes an $N_c \times N_\mu$ rectangular matrix $\tilde{v}_c$. The matrix equation read

$$\begin{bmatrix} H_{int} - E\mathbb{1} - \tilde{v}_c \frac{1}{-E+t_c e^{ikc}} (\tilde{v}_c)^T & (\vec{v}_r)^T \\ \vec{v}_r & -E \end{bmatrix} \begin{pmatrix} \vec{x}_{int} \\ x_a \end{pmatrix} = \begin{pmatrix} \vec{0} \\ -t_a \end{pmatrix}. \tag{29}$$

The equation is solved for x_a, r, and then the wave function ϕ, as before. The outgoing fluxes are computed from $\vec{x}_{int}$ which is given by

$$\vec{x}_{c,i} = \frac{1}{-E + t_{c,i}e^{ik_{c,i}}} \sum_j \tilde{v}_{c,ij}\vec{x}_{aj}. \tag{30}$$

In fact, it is not necessary to treat the exit channels in any detail. The imaginary part of the term $v_{\mu c}^2/(-E + t_c e^{ik_c}) = \Gamma_{mu,c}/2$ that is added to the diagonal energy of state μ gives the decay rate of that state,

$$W_{\mu,c} = |\phi_\mu|^2 \Gamma_{mu,c}. \tag{31}$$

6. **More elegant formulations**

We mention here the formulations of reaction theory focussing on the internal Hamiltonian of the combined projectile-target system, leaving the coupling to the incoming and outgoing channels to be determined separately. Most fundamental is the S-matrix formulation. All channels are treated on an equal footing, so the entire S-matrix is calculated by standard linear algebra operations.

The quantities that are represented in a matrix form are:

–the Hamiltonian H of the internal states, an $N_\mu \times N_\mu$ matrix;

–an energy shift matrix Δ of the same dimension, arising from the couplings to the channel space;

–the reduced coupling widths $\tilde{\gamma}$, an $N_\mu \times N_c$ matrix.

The reduced-width matrix is related to the decay width of a state μ into a channel c by

$$\Gamma_{\mu,c} = 2\gamma_{\mu,c}^2. \tag{32}$$

The expression for S in terms of these quantities is [2]

$$S = 1 - 2\tilde{\gamma}^T G \tilde{\gamma}. \tag{33}$$

where

$$G = (E - H - \Delta - \tilde{\gamma}\tilde{\gamma}^T)^{-1} \tag{34}$$

Application of this formula requires the inversion of a complex matrix; that is no more difficult than inversion of a real matrix.

It sometimes convenient to study the internal Hamiltonian in isolation without built-in couplings inherent in Eq. (33). This is the motivation for the K-matrix formulation [3]. The K-matrix an $N_c \times N_c$ matrix defined as

$$K = \tilde{\gamma}^T (E - H)^{-1} \tilde{\gamma} \tag{35}$$

and the derived S-matrix

$$S = (1 - iK)(1 + iK)^{-1}. \tag{36}$$

Below is a Mathematica script to work this out for the case of a single internal state and two channels. The variables are $a = \gamma_a/(-E + E_r)^{1/2}$ and $b = \gamma_b/(-E + E_r)^{1/2}$.

```
K = {{a^2,a b},{a b,b^2}}
unit = {{1,0},{0,1}}
num = (unit- I K)
den = Inverse[ unit + I K]
S = num.den
Saa = Simplify[S[[1]][[1]]]
Sab = Simplify[S[[1]][[2]]]
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The elements in the first row of the S-matrix are seen to be:

$$S_{aa} = \frac{1 - ia^2 + ib^2}{1 + i(a^2 + b^2)} \tag{37}$$

$$S_{ab} = \frac{-2iab}{1 + i(a^2 + b^2)}. \tag{38}$$

Note that complete transmission from one channel to the other requires the quantities $|a|$ and $|b|$ are equal and taking the limit $|a|, |b| \to \infty$. It can easily be shown that Eq. (35-36) are equivalent to the formulas derived from fluxes associated with the wave function. We start with an expression for r for the two-channel, one-resonance scattering derivable from Eq. (25)

$$r = \frac{1 - e^{-ik_a} \frac{v_a^2/t_a}{E - E_r - v_b^2/(-E + t_b e^{ik_b})}}{1 - e^{+ik_a} \frac{v_a^2/t_a}{E - E_r - v_b^2/(-E + t_b e^{ik_b})}}. \tag{39}$$

Note the $-E + t_b e^{ik_b} = -t_b e^{-ik_b}$. Then we can write r as

$$r = \frac{E - E_r - e^{-ik_a} v_a^2/t_b - e^{ik_b} v_b^2/t_b}{E - E_r - e^{ik_a} v_a^2/t_b - e^{ik_b} v_b^2/t_b}. \tag{40}$$

Apart from the level shifts, this is identical to Eq. (37). The γ in the K-matrix is identified with quantities in the discrete basis according to

$$\gamma_c^2 = \Gamma_c/2 = |U_p|^2 v_r^2/4t_a \sin(k_a). \tag{41}$$

Finally, there is an elegant formulation of reaction theory [4, 5] to deliver the transmission factors to the final channels $T_{ab} \equiv |S_{ab}|^2$. They may be calculated by the trace formula

$$T_{ab} = \mathrm{Tr}(\Gamma_a G \Gamma_b G^\dagger). \tag{42}$$

Here all factors are $N_\mu \times N_\mu$ matrices in the internal Hamiltonian space.

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