AN APPROACH TO THE COMPUTATION OF FEW/MANY–BODY MULTICHANNEL REACTIONS

V.D. Efros

National Research Centre "Kurchatov Institute", Moscow

1. GENERAL SCHEME

The conventional approach is to construct the continuum spectrum states (Ψ_γ). The specification of open reaction channels is required to get Ψ_γ. Appropriate at low energies. Impractical at higher energies and larger number of particles.

The approach presented below: reaction channels emerge at the kinematics level only, when a dynamics calculation is already done. Instead of Ψ_γ, quantities to be extracted from a dynamics calculation are response–like functions

$$R(E) = \sum_n \langle Q'|\Psi_n\rangle\langle\Psi_n|Q\rangle\delta(E-E_n) + \sum\!\!\!\!\!\!\int d\gamma \langle Q'|\Psi_\gamma\rangle\langle\Psi_\gamma|Q\rangle\delta(E-E_\gamma),$$

$$H\Psi_n = E_n\Psi_n, \quad \langle\Psi_n|\Psi_{n'}\rangle = \delta_{nn'}, \quad H\Psi_\gamma = E_\gamma\Psi_\gamma, \quad \langle\Psi_\gamma|\Psi_{\gamma'}\rangle = \delta(\gamma-\gamma').$$

Let us express reaction observables in terms of quantities having the above structure. Consider strong–

interaction induced reactions, $\alpha \to \beta$:

$$T_{\beta\alpha} = T^{Born}_{\beta\alpha} + \langle \bar{\phi}_\beta(E)|(E - H + i\epsilon)^{-1}|\bar{\phi}_\alpha(E)\rangle,$$

$$\bar{\phi}_{\alpha,\beta}(E) = (H - E)\mathcal{A}\phi_{\alpha,\beta}(E) = \mathcal{A}(H - E)\phi_{\alpha,\beta}(E) = \mathcal{A}V^{res}_{\alpha,\beta}\phi_{\alpha,\beta},$$

$$(\mathcal{A}^2 = \mathcal{A}), \qquad T^{Born}_{\beta\alpha} = \langle \phi_\beta|\bar{\phi}_\alpha\rangle = \langle \bar{\phi}_\beta|\phi_\alpha\rangle.$$

The Coulomb interaction is disregarded here.

The non–Born contribution may be presented as

$$\int dE' R_{\beta\alpha}(E')(E - E' + i\epsilon)^{-1}$$

where $R_{\beta\alpha}(E')$ **is just of the same structure as** $R(E)$ **above with** $E \to E'$, $Q \to \bar{\phi}_\alpha(E)$, $Q' \to \bar{\phi}_\beta(E)$.

(Exclusive) reactions induced by a perturbation,

$$\langle \Psi^-_\beta|O|\Psi_0\rangle = \langle \phi_\beta|O|\Psi_0\rangle + \langle \bar{\phi}_\beta|(E - H + i\epsilon)^{-1}|O\Psi_0\rangle.$$

The second contribution is expressed in terms of a response–like function of the same structure as above with $\bar{\phi}_\alpha \to O\Psi_0$.

Thus the question is how the response–like functions may be obtained. An easy task is the sum–rule calculation. Since

$$\sum_n |\Psi_n\rangle\langle\Psi_n| + \sum\!\!\!\!\!\!\int d\gamma |\Psi_\gamma\rangle\langle\Psi_\gamma| = I,$$

one has

$$\int dE R(E) = \langle Q'|Q\rangle.$$

(recall)

$$R(E) = \sum_n \langle Q'|\Psi_n\rangle\langle\Psi_n|Q\rangle\delta(E-E_n) + \sum\!\!\!\!\!\!\int d\gamma \langle Q'|\Psi_\gamma\rangle\langle\Psi_\gamma|Q\rangle\delta(E-E_\gamma).$$

"Generalized sum rules" depending on a parameter:

$$\int dE\, K(\sigma, E)R(E) = \sum_n \langle Q'|K(\sigma, H)|\Psi_n\rangle\langle\Psi_n|Q\rangle\delta(E-E_n)$$

$$+ \sum\!\!\!\!\!\!\int d\gamma \langle Q'|K(\sigma, H)|\Psi_\gamma\rangle\langle\Psi_\gamma|Q\rangle\delta(E-E_\gamma) = \langle Q'|K(\sigma, H)|Q\rangle \equiv \Phi(\sigma).$$

Thus, the integral equation (with the inclusion of discrete contributions) of the form

$$\Phi(\sigma) = \int dE\, K(\sigma, E)R(E)$$

is employed to determine $R(E)$. A general approach to its solution:

$$R(E) \to R_{trial}(E, \{c\}), \qquad \int dE\, K(\sigma, E)R_{trial}(E, \{c\}) = \Phi_{trial}(\sigma, \{c\})$$

$$\int d\sigma\, w(\sigma)[\Phi(\sigma) - \Phi_{trial}(\sigma, \{c\})]^2 = \min_{\{c\}}.$$

The R_n discrete contributions may be either included to the $\{c\}$ set or calculated separately.

2. CALCULATING THE TRANSFORMS. SPECIFIC KERNELS

Now consider the calculation of the input $\langle Q'|K(\sigma,H)|Q\rangle$ to the integral equation. If one is able to diagonalize the Hamiltonian in a sufficiently big subspace $\{\varphi_n\}$ of localized functions, $\langle\varphi_n|H|\varphi_{n'}\rangle = \delta_{nn'}$, then

$$\langle Q'|K(\sigma,H)|Q\rangle \simeq \sum_n \langle Q'|\varphi_n\rangle K(\sigma,E_n)\langle\varphi_n|Q\rangle.$$

Ways to proceed for some particular kernels without the diagonalization of the Hamiltonian. Consider the Stieltjes transform, $K(\sigma,E)=(\sigma+E)^{-1}$. One has

$$\langle Q'|K(\sigma,H)|Q\rangle = \langle Q'|(\sigma+H)^{-1}|Q\rangle = \langle Q'|\tilde{\Psi}(\sigma)\rangle,$$

$$(H+\sigma)\tilde{\Psi} = Q.$$

This is the dynamics problem to be solved. $\tilde{\Psi}$ is localized $(\sigma > -|E_0|)$. In the case of strong–interaction induced reactions the Coulomb interaction in the entrance channel may be accounted for.

The "Lorentz transform": $K(\sigma,E) = [(\sigma-E)^2+\Gamma^2]^{-1}$. Writing

$$\frac{1}{(\sigma-E)^2+\Gamma^2} = \frac{1}{2i\Gamma}\left[\frac{1}{(\sigma-E)-i\Gamma} - \frac{1}{(\sigma-E)+i\Gamma}\right]$$

the transform is calculated in terms of two Stieltjes–type transforms,

$$\langle Q'|K(\sigma,H)|Q\rangle = \frac{1}{2i\Gamma}\langle Q'|(\tilde{\Psi}_+ - \tilde{\Psi}_-)\rangle,$$

$$(H - \sigma \pm i\Gamma)\tilde{\Psi}_\pm = Q.$$

The Laplace transform: $K(\sigma,E) = e^{-\sigma E}$. **The input** $\langle Q'|e^{-\sigma H}|Q\rangle$ **may be calculated with the GFMC method.**

3. INVERSION OF THE TRANSFORMS

Let us omit the discrete contributions to $R(E)$ for the presentation simplicity. Then one has the integral equation of the first kind

$$\Phi(\sigma) = \int_{E_{thr}}^{\infty} dE\, K(\sigma,E)R(E)$$

to determine $R(E)$. At a given Φ the solution is unique but small variations of Φ may cause large variations of R of a high frequency. Small variations of Φ may also lead to narrow peaks in R with large amplitudes provided that contributions of the peaks to the integral are negligible. (So called "ill–posed problem".)

A conventional way to perform the inversion that was

employed in actual calculations:

$$R(E) \simeq \sum_{n=1}^{n_{max}} c_n \chi_n(E).$$

The c_n coefficients are determined by fitting to $\Phi(\sigma)$ as discussed above. The basis functions represent the threshold behavior of $R(E)$ when known. The n_{max} value should be sufficiently large to represent the true $R(E)$ properly and sufficiently small to prevent the appearance of false oscillations or narrow peaks in $R(E)$. Whether these two conditions are compatible depends on the accuracy in $\Phi(\sigma)$. The "convergence" criterion: results should be stable in some range of n_{max}.

A new way to perform the inversion (under study). At a given Φ, the accuracy in R may be improved when an additional information on R is incorporated in the inversion algorithm. The number of narrow maxima and minima of R, as taken from experiment or a reasonable guess, may be adopted as such an information. The equation is solved at the condition imposed that R possesses a given number of maxima and minima. This

removes false high–frequency oscillations. The integral equation is rewritten in the form of such an equation for the derivative of R which derivative thus should possess a given number of zeros. The most general expression for such a derivative is written. It includes an expansion like $\exp \sum_{n=1}^{\infty} c_n \psi_n(E)$. A set of the c_n parameters retained along with a finite number of other parameters entering this expression is fitted to $\Phi(\sigma)$. It has been proven that, when the number of maxima and minima is taken to be correct, small variations of Φ cannot lead to large variations of R (which is a well–posed problem) at least beyond close proximities of maxima and minima of R.

4. REFERENCES AND SOME STUDIES DONE SO FAR WITH THIS APPROACH

Integral transforms (continuous sets of sum rules) of observable response functions. (No inversion.)

V.D.E., Ukr. Fiz. Zh. **25**, 907 (1980). (The Stiltjes transform.)

D. Thirumalai, B.J. Berne, J. Chem. Phys. **79**, 5029 (1983). (The Laplace transform.)

A related approach: the method of moments to calcu-

late observable response functions

W.P. Reinhardt, P.W. Langhoff, in *Theory of Applications of Moment Methods in Many–Fermion Systems*, ed. B.J. Dalton *et al*, Plenum, N.Y., 1980.

The method for the computation of general type reactions. Inversions of the transforms.

V.D.E., Sov. J. Nucl. Phys. **41** 949 (1985). (The Stiltjes–type transforms were employed.)

The Lorentz transform

V.D.E., W. Leidemann, G. Orlandini, PLB **338** 130 (1994).

Some developments and a review

V.D.E. Phys. At. Nucl., **62** 1833 (1999).

A review

V.D.E., W. Leidemann, G. Orlandini, N. Barnea, J. Phys. G: Nucl. Part. Phys. **34** R459 (2007).

The alternative inversion method

V.D.E., PRE **86** 016704 (2012).

Studies of observable (inclusive) responses

Lorentz transform:

Photodisintegration of the ^{3}H, ^{3}He and ^{4}He nuclei

Longitudinal and transverse (e, e') response functions of the ^{3}H, ^{3}He and ^{4}He nuclei including relativistic and Δ isobar effects in the nuclear sector

The spectral function of the ^{4}He nucleus

Inclusive neutrino reactions on the ^{4}He nucleus

(H. Arenhövel, S. Bacca, N. Barnea, V.D.E., D. Gazit, W. Leidemann, P. Navratil, G. Orlandini, S. Quaglioni, E.L. Tomusiak, L. Yuan, et. al.)

Some activities as to heavier nuclei

(S. Bacca, N. Barnea, W. Leidemann, G. Orlandini, et. al.)

Laplace transform:

Condensed matter physics

Electromagnetic and neutral–weak responses of the ^{4}He and ^{12}C nuclei: GFMC

Studies of exclusive perturbation–induced reactions

d$(e, e'$p): (a test of the method) A. La Piana, W. Leidemann, NPA **677**, 423 (2000)

^{4}He(γ,p)^{3}H and ^{4}He(γ,n)^{3}He: S. Quaglioni, N. Barnea, W. Leidemann, G. Orlandini, V.D.E, PRC **69**, 044002 (2004)

^{4}He$(e, e'$p$)^3$H: S. Quaglioni, V.D.E., W. Leidemann, G. Orlandini, PRC **72**, 064002 (2005)

^{4}He(γ,p)^{3}H and ^{4}He(γ,n)^{3}He: N. Nevo Dinur, W. Leidemann, N. Barnea, FBS **55**, 997 (2014)

No studies for strong–interaction induced reactions.

5. ACCURACY TESTS PERFORMED

In particular, a benchmark study of the three–nucleon photodisintegration.

A test of the method:

Comparison of the calculated cross section for photodisintegration of ^{3}H (NPA, 2001) with the subsequent Bohum–Krakow group Faddeev calculation (NPA, 2002). The AV18 NN interaction.