Single-step and coupled-channels calculations of pion inelastic scattering

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We discuss, in a collective framework, single-step and coupled-channels distorted-wave calculations for inelastic scattering of pions from nuclei. Two frequently used codes are compared and contrasted.
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I. INTRODUCTION

The distorted-wave impulse-approximation (DWIA) code DWPI [1] is widely used to calculate cross sections for pion inelastic scattering. Coupled-channels calculations are frequently carried out with the code NEWCHOP, a modified version of CHOPIN [2]. In CHOPIN (and hence in NEWCHOP), the initial, intermediate, and final states are teated explicitly as rotational in character — indeed all three are treated as members of the same rotational band, with bandhead angular momentum projection K. In DWPI, no such assumption is made. Rather, the language is more in the spirit of a vibrational collective model. The two codes have been used extensively for predictions of scattering cross sections in inelastic π-nucleus scattering, and fitting of data for the extraction of the collective strength parameter β, or equivalently the reduced transition probability $B(E\lambda)$. Care must be exercised when comparing the two codes, especially for calculations in which the initial state has nonzero spin.

In this work, we wish to resolve the ambiguities regarding the two codes, and show how to use them correctly for data analysis. In Sec. II we present the correct formulas for the transition matrix element and reduced transition probability in the vibrational and rotational collective models (VCM, RCM) and compare them with the formulas used by the two codes. We also define the appropriate value of the parameter β in order that both codes perform calculations in either model correctly, and point to the kind of previous calculations which need to be reconsidered. In Sec. III we show one- and two-step calculations compared to data, and provide examples of data analysis which yield the strengths of the various multipoles contributing to a given transition.

II. REVIEW OF THE COLLECTIVE MODELS

The two major sources of ambiguity in using the two codes are the various versions of the Wigner-Eckart theorem currently used in the literature, as represented — for example — by Satchler [3] and Edmonds [4], as well as the various definitions of the strength parameter β used in different formulations of the collective models. The physical observables affected by such ambiguities are the transition amplitude and the reduced transition probability. It is appropriate, therefore, to begin by defining the parameter β in the context of both the VCM and the RCM as used by the codes. We will follow the notation of [1], the source of the code DWPI, and often refer to fomulas derived there.

We remind the reader that an expansion of the nuclear radius

$$R = R_0\left(1 + \sum_{\lambda\mu} \alpha^*_{\lambda\mu} Y_{\lambda\mu}(\hat{\mathbf{r}})\right) \tag{1}$$

is typically used in parametrizations of the collective nuclear density [5]

$$\rho(\mathbf{r}, R) = \rho(\mathbf{r}, R_0) + \delta\rho(\mathbf{r}, R_0) \ , \tag{2}$$

where $\rho(\mathbf{r}, R_0)$ and $\delta\rho(\mathbf{r}, R_0)$ are the elastic and transition densities, respectively. We use a normalization of the ground-state density $\rho(\mathbf{r}, R_0)$ such that

$$\int d^3r \ \rho(\mathbf{r}, R_0) = 1 \ , \tag{3}$$

as in [1]. The multipole expansion of the collective transition density used throughout this work is

$$\begin{aligned}\delta\rho(\mathbf{r}, R_0) &= \left(-R_0 \frac{\partial\rho}{\partial r}\Big|_{R=R_0}\right) \sum_{\lambda\mu} \alpha^*_{\lambda\mu} Y_{\lambda\mu}(\hat{\mathbf{r}}) \\ &= f(r) \sum_{\lambda\mu} \alpha^*_{\lambda\mu} Y_{\lambda\mu}(\hat{\mathbf{r}}) \ ,\end{aligned} \tag{4}$$

where λ is the transferred angular momentum and $\alpha_{\lambda\mu}$ are model-dependent multipole coefficients. These coefficients are spherical tensors that have the same properties under rotations as the spherical harmonics. The parameter β is introduced through them. In the VCM, $\alpha_{\lambda\mu}$ is defined in terms of phonon creation and annihilation operators coupled to λ, μ:

$$\alpha_{\lambda\mu} = \frac{1}{\sqrt{2\lambda+1}} \left[\tilde{b}_{\lambda\mu} + (-)^\mu \tilde{b}^\dagger_{\lambda-\mu}\right]. \tag{5}$$

We point to the difference between (5) and formula (7) of [1]. The parameter β_λ, or strength of the multipole λ, is related to the reduced matrix element of these coefficients between the states of interest:

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$$\langle I_f \| \alpha_\lambda \| I_i \rangle = \beta_\lambda \sqrt{\frac{(2I_i+1)(2I_f+1)}{2\lambda+1}} . \quad (6)$$

The reduced matrix element in (6) is in the Edmonds convention.

In the RCM, one does not speak of phonon excitations, but rather of nuclear collective deformations. In this language, the coefficients $\alpha_{\lambda\mu}$ are defined by [6]

$$\alpha_{\lambda\mu} = \beta_\lambda \sqrt{\frac{4\pi}{2\lambda+1}} Y_{\lambda\mu}(\hat{\Omega}) , \quad (7)$$

where $\hat{\Omega}$ is the collective nuclear orientation.

Thus, we have the connection of the multipole strengths β_λ with the transition density, as one can check by substituting the coefficients $\alpha_{\lambda\mu}$ in the VCM or RCM, formula (5) or (7) respectively, into (4). Subsequently, one proceeds to build the optical potential and to take matrix elements of the transition density between states of interest. Bypassing intermediate steps, we provide the correct formulas for the transition matrix elements in the VCM and RCM obtained by using the multipole strengths β_λ as defined above. In the VCM, we have

$$T^{J\lambda}_{l_f I_f; l_i I_i} = \beta_\lambda i^{l_i - l_f} (-)^{J+\lambda} \sqrt{\frac{(2l_f+1)(2l_i+1)(2I_f+1)(2I_i+1)}{4\pi}} \times \begin{pmatrix} l_f & \lambda & l_i \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_i & I_i & J \\ I_f & l_f & \lambda \end{Bmatrix} [A_1 I_1 + A_2 I_2 + A_3 I_3]_{l_f l_i \lambda} , \quad (8)$$

and in the RCM

$$T^{J\lambda}_{l_f I_f; l_i I_i} = \beta_\lambda \delta_{K_i K_f} i^{l_i - l_f} (-)^{J+\lambda-K_i} \sqrt{\frac{(2l_f+1)(2l_i+1)(2I_f+1)(2I_i+1)(2\lambda+1)}{4\pi}} \times \begin{pmatrix} l_f & \lambda & l_i \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} I_f & \lambda & I_i \\ -K_i & 0 & K_i \end{pmatrix} \begin{Bmatrix} l_i & I_i & J \\ I_f & l_f & \lambda \end{Bmatrix} [A_1 I_1 + A_2 I_2 + A_3 I_3]_{l_f l_i \lambda} . \quad (9)$$

In (8) and (9), the angular momenta of the π and the nucleon are denoted by l, I, with subscripts i, f indicating initial and final states. These couple to J, the channel angular momentum. The angular momentum transfer and the spin projection along the axis of symmetry in the deformed nucleus are represented by λ and K, respectively. The radial integrals I_1 and I_2 and the coefficients A_1, A_2, A_3 are as in [1] and [7]. The parentheses and curly brackets are $3J$ and $6J$ symbols. The integral I_3 is given by

$$I_3 = \int dr\, u^{-*}_{l_i} \left(\frac{\partial^2 f(r)}{\partial r^2} + \frac{2}{r} \frac{\partial f(r)}{\partial r} - \frac{\lambda(\lambda+1)}{r^2} f(r) \right) u^{+}_{l_f} , \quad (10)$$

where $f(r)$ in I_3 is the same as in (4). Note that (10) differs from (18) of [1] in the sign of the second term. The correct formula (10), however, is implemented in the code.

It should be noted that (8) has an extra factor of $\sqrt{2I_i+1}$ relative to Eq. (15) of Ref. [1], the source of DWPI. This factor is required in order to guarantee the invariance of (8) under interchange of initial and final states. The absence of this factor in the formula used by DWPI results in incorrect calculation of matrix elements and cross sections when the initial nuclear state has nonzero spin. This problem can be easily detected by considering the ratio of cross sections of a forward to a backward calculation by DWPI: Kinematical corrections notwithstanding — small in any case for low excitations — detailed balance requires that

$$\frac{\sigma(J_i \to J_f)}{\sigma(J_f \to J_i)} = \frac{2J_f+1}{2J_i+1} . \quad (11)$$

For $J_i = 0$ in particular, (11) yields

$$\frac{\sigma(0 \to J)}{\sigma(J \to 0)} = 2J+1 . \quad (12)$$

Results of DWPI give instead

$$\sigma(J_i \to J_f) = \frac{(2J_f+1)}{(2J_i+1)(2\lambda+1)} \sigma(0 \to \lambda) , \quad (13)$$

so that for $J_i = 0$,

$$\frac{\sigma(0 \to J)}{\sigma(J \to 0)} = (2J+1)^2 . \quad (14)$$

This is a consequence of the fact that whereas $\sigma(0 \to J)$ is calculated correctly, $\sigma(J \to 0)$ is reduced by a factor of $(2J+1)$.

The code NEWCHOP uses (9) for the evaluation of the transition matrix element and the cross section. However, it has been used frequently in the past for coupled-channels calculations of transitions between spherically symmetric states, where K is an irrelevant quantum number and (8) ought to be used instead. Comparison between (8) and (9) shows that simply setting $K = 0$ does not make the VCM and RCM matrix elements equivalent, unless at least one of I_i, I_f is zero. Consequently, calculations by NEWCHOP between spherically symmetric states done in this fashion, have been correct only for transitions which involve at least one state of zero spin in each step.

The reduced transition probability $B(E\lambda)$ is defined

by [8]

$$B(E\lambda, I_i \rightarrow I_f) = \frac{|\mathcal{M}_p(E\lambda)|^2}{2I_i+1} = \frac{|\langle I_f||\tilde{Q}_\lambda||I_i\rangle|^2}{2I_i+1} , \quad (15)$$

where $\tilde{Q}_\lambda$ is the electric multipole operator which also depends on the transition density. Note that $\mathcal{M}_p(E\lambda)$, the reduced matrix element of the electric multipole operator between states of interest in the Edmonds convention, is invariant upon interchange of the initial and the final state.

One can retrace the steps described earlier which would have to be followed for the derivation of the transition matrix element, and become convinced that the reduced transition probability will be different for the VCM and the RCM, and will depend on the multipole strengths β_λ. One thus arrives at the following formulas, appropriate for the two collective models:

$$B(E\lambda, I_i \rightarrow I_f) = \frac{2I_f+1}{2\lambda+1}\left(Z\beta_\lambda \int dr\, r^{\lambda+2} f(r)\right)^2 \quad (16)$$

in the VCM, and

$$B(E\lambda, I_i \rightarrow I_f) = \delta_{K_i,K_f}(2I_f+1)\left(Z\beta_\lambda \int dr\, r^{\lambda+2} f(r)\right)^2 \left|\begin{pmatrix} I_f & \lambda & I_i \\ K_i & 0 & -K_i \end{pmatrix}\right|^2 \quad (17)$$

in the RCM, where $f(r)$ is as in (4) and Z is the charge. Hence, according to (15), we have

$$M_p(E\lambda) = \sqrt{\frac{(2I_i+1)(2I_f+1)}{2\lambda+1}}\left(Z\beta_\lambda \int dr\, r^{\lambda+2} f(r)\right) \quad (18)$$

in the VCM, and

$$M_p(E\lambda) = \delta_{K_i,K_f}\sqrt{(2I_i+1)(2I_f+1)}\left(Z\beta_\lambda \int dr\, r^{\lambda+2} f(r)\right)\begin{pmatrix} I_f & \lambda & I_i \\ K_i & 0 & -K_i \end{pmatrix} \quad (19)$$

in the RCM. Substitution of Z by N yields the $B(N\lambda)$'s and the M_n's. The code DWPI also calculates the $B(E,N\lambda)$'s incorrectly for many cases. The old version of DWPI calculates $B(E,N\lambda)$'s in units of $e^2\,\mathrm{fm}^{2\lambda}$ as well as in W.u. (Weisskopf units). Various errors resulted in these being correct only for $0 \rightarrow J$ transitions in $e^2\,\mathrm{fm}^{2\lambda}$ and $J \rightarrow 0$ transitions in W.u. For the derivation of the $\mathcal{M}_{p,n}$'s in previous analyses, Eq. (15) was used, and it was assumed that the $B(E,N\lambda)$ ↑'s were correct in units of $e^2\,\mathrm{fm}^{2\lambda}$. For identical cross sections between our modified and the old version of DWPI, the relation $\beta_{\mathrm{old}}^{\mathrm{DWPI}} = \beta_{\mathrm{new}}^{\mathrm{DWPI}}\sqrt{2J_i+1}$ must hold. The code NEWCHOP does not calculate the $B(E,N\text{-}\lambda)$'s. For identical cross sections in calculations involving spherically symmetric nuclei with NEWCHOP, $\beta_{\mathrm{old}}^{\mathrm{NEWCHOP}}/\beta_{\mathrm{new}}^{\mathrm{NEWCHOP}}$ must be in the same ratio as $T^{J\lambda}_{l_f I_f; l_i I_i}(\mathrm{VCM})/T^{J\lambda}_{l_f I_f; l_i I_i}(\mathrm{RCM})$ of Eqs. (8) and (9).

III. NUMERICAL RESULTS

We have thus presented the correct formulas for the transition matrix element and the reduced transition probability in the VCM and RCM and have shown how they should be used by the codes DWPI and NEWCHOP. We have created modified versions of the two codes which

TABLE I. Examples of calculation of $\mathcal{M}_p$ and $\mathcal{M}_n$, the reduced matrix elements of electromagnetic operators of known multipolarity for protons and neutrons, using our modified versions of the codes in the VCM.

Target	E_x (MeV)	J_i^π	J_f^π	$E\lambda$	β_p	β_n	Pion scattering ($e\,\mathrm{fm}^\lambda$) $\mathcal{M}_p$	Pion scattering ($e\,\mathrm{fm}^\lambda$) $\mathcal{M}_n$	Electromagnetic ($e\,\mathrm{fm}^\lambda$) $\mathcal{M}_p$	Electromagnetic ($e\,\mathrm{fm}^\lambda$) $\mathcal{M}_n$
Modified DWPI calculations in the VCM										
^{39}K [a]	2.52	$\frac{3}{2}^+$	$\frac{1}{2}^+$	$E2$	0.145±0.009	0.066±0.004	13.9±0.9	6.6±0.4	8.2±1.5 [b]	≤8.2 [c]
^{39}K [a]	3.02	$\frac{3}{2}^+$	$\frac{3}{2}^-$	$E3$	0.210±0.014	0.170±0.011	110.0±7.1	93.9±6.1	118.7±91.2 [b]	245.0 ± 110.8 [c]
Modified NEWCHOP calculations in the VCM										
^{44}Ca [d]	1.16	0^+	2^+	$E2$	0.264±0.024	0.271±0.024	20.7±1.9	28.4±2.5	21.3±0.7 [b]	
^{44}Ca [d]	2.28	0^+	4^+	$E4$	0.112±0.010	0.050±0.005	190.5±17.2	118.7±10.7	190.5±5.6 [e]	
^{44}Ca [d]	2.28	2^+	4^+	$E2$	−0.165±0.027 [f]	0.123±0.020	−38.6±6.4 [f]	38.6±6.4	38.6±6.4 [b]	

[a] Data from Ref. [9]. Pion M_p and M_n from present work.

[b] Reference [10].

[c] Reference [11].

[d] Data and matrix elements from Ref. [12].

[e] References [13,14].

[f] Sign explained in Ref. [12].

TABLE II. Input parameters that result in the same cross sections as those of Table I, but using the unmodified versions of DWPI and NEWCHOP.

Target	E_x (MeV)	J_i^π	J_f^π	β_p	β_n
Old DWPI calculations					
^{39}K	2.52	$\frac{3}{2}^+$	$\frac{1}{2}^+$	0.290±0.018	0.132±0.008
^{39}K	3.02	$\frac{3}{2}^+$	$\frac{3}{2}^-$	0.420±0.028	0.340±0.022
Old NEWCHOP calculations,[a] setting $K = 0$					
^{44}Ca	1.16	0^+	2^+	0.264±0.024	0.271±0.024
^{44}Ca	2.28	0^+	4^+	0.112±0.010	0.050±0.005
^{44}Ca	2.28	2^+	4^+	−0.309±0.051	0.230±0.037

[a]See text in Sec. II, following (14).

have as a standard option the choice of either collective model, and calculate $B(E\lambda)$ for each step.

We now present two examples of past incorrect usage of the codes: one case involves single-step calculations on a $J_i \neq 0$ target (viz. ^{39}K), with DWPI; the other involves coupled-channels calculations with NEWCHOP in ^{44}Ca. The results of these calculations, using our modified versions of the codes, are shown in Table I. The values of the strength parameter β, which reproduce our calculated cross sections using the older incorrect versions, are shown in Table II.

For ^{39}K, we have chosen one quadrupole and one octupole transition (see Table I). We have simultaneously varied β_p and β_n (equivalently, M_p and M_n) to fit the data. For the $\frac{1}{2}^+$ state at 2.52 MeV, and the $\frac{3}{2}^-$ state at 3.02 MeV, the data and calculations are plotted in Fig. 1. The curves are for $\lambda = 2$, 3 collective transitions, as in [9]. Quality of fit is almost as in the original reference. But our goal here is not to search for the best fit, but simply to obtain correct M_p's and M_n's. They are listed in Table I. We note that they differ from those of Ref. [9], primarily by a factor $[(2J_f + 1)/(2\lambda + 1)]^{1/2}$. It is likely that many (π, π') results for odd-A targets in the literature suffer from a similar mistake.

The coupled-channels examples are for ^{44}Ca(π^+, π^+), leading to the 2^+, 0^+, and 4^+ excited states at 1.16, 1.88, and 2.28 MeV, respectively. In these examples we use the values of M_p and M_n from [12]; our results for the $0^+_{g.s.} \rightarrow 2^+ \rightarrow 0^+_2$ coupled-channels calculation, and the direct transition $0^+_{g.s.} \rightarrow 0^+_2$, are identical to those shown in Fig. 4 of [12], as expected from the discussion of the previous section for transitions involving at least one state of zero spin. These are therefore not shown here. Our calculation for the coupled-channels transition $0^+_{g.s.} \rightarrow 2^+ \rightarrow 4^+$, however, differs from that of [12] in both shape and magnitude. The difference in shape is independent of our changes to NEWCHOP; rather, in an unrelated error, the shape of the coupled-

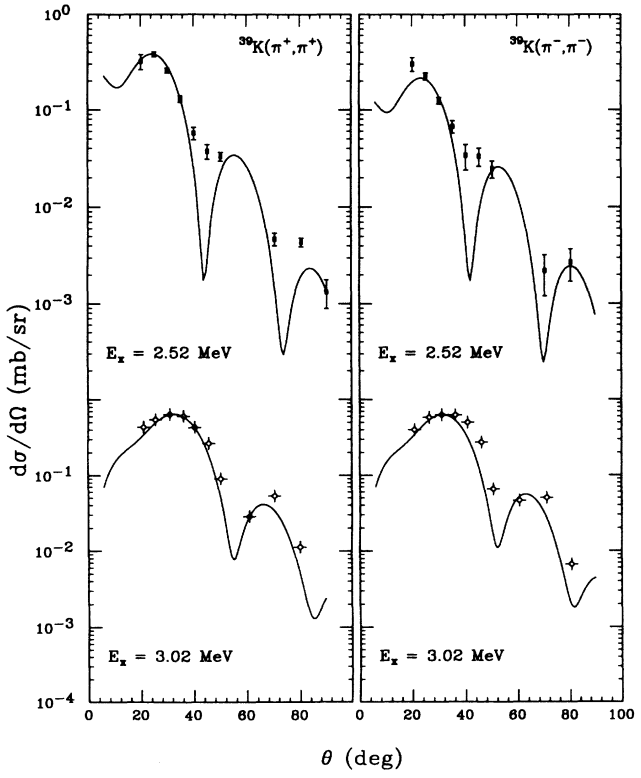

FIG. 1. Pion inelastic scattering on ^{39}K leading to the lowest $\frac{1}{2}^+$ ($E_x = 2.52$ MeV) and $\frac{3}{2}^-$ ($E_x = 3.02$ MeV) states. The solid curves represent single-step DWPI calculations with parameters from Table I. The data, density parameters, and energy shift used in the calculations are from [9]. Whenever no error bars are indicated, the data were read from Fig. 2 of [9].

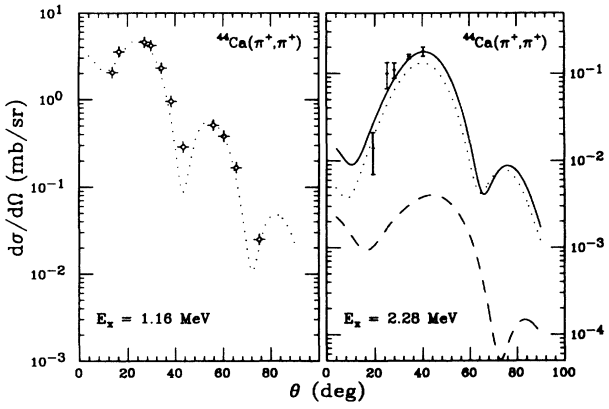

FIG. 2. Pion inelastic scattering from ^{44}Ca to the lowest 2^+ ($E_x = 1.16$ MeV) and 4^+ ($E_x = 2.28$ MeV) states. The curves represent NEWCHOP calculations with the parameters of Table I. Dotted curves are one-step calculations, with $\lambda = J_f$. The dashed curve is from a coupled-channels calculation, involving coupling of the target g.s., the first 2^+, and the final 4^+ states. The solid curve is obtained by combining the single-step and coupled-channels calculations. The data, density parameters, and energy shift used in the calculation are from [12]. The data for $E_x = 1.16$ MeV were read from Fig. 2 of [12], thus error bars are not indicated.

channels calculation in [12] corresponds to the transition $0^+_{g.s.} \rightarrow 2^+ \rightarrow 2^+$, instead. Single-step, coupled-channels, and total calculations for $^{44}Ca(\pi^+, \pi^+)$ are displayed in Fig. 2.

We have thus resolved past ambiguities regarding the meaning of the multipole strength, β_λ, in calculations by the codes DWPI and NEWCHOP. We have provided the correct expressions for the transition matrix elements and $B(E\lambda)$'s, consistent with the VCM and the RCM, and discussed the extraction of β_λ's from pion inelastic scattering data.

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