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The Multipole Expansion of Realistic Effective Interactions in Nuclei*

When a realistic nucleon–nucleon interaction with a repulsive core is otherwise attractive, a fair approximation to the corresponding reaction matrix or effective interaction is obtained by using the Moszkowski–Scott separation method [1] in lowest order, which gives just the long-range part of the free two-nucleon interaction. This results in an exponential-like outer region with a cutoff at the separation distance d. Pinkston and Philpott suggested [2] the use of a sum of cutoff Yukawa terms to fit such a truncated potential. The effective potential, or t matrix, for two interacting particles separated by a distance r_{12} is written as

$$t(r_{12}) = -V \sum_{n} A_n g(n\alpha r_{12}), \tag{1}$$

where n is an integer, $r_{12} = | \mathbf{r}_1 - \mathbf{r}_2 | = (r_1{}^2 + r_2{}^2 - 2r_1 r_2 \cos \theta_{12})^{1/2}$, and

$$\begin{aligned} g(\beta r_{12}) &= e^{-\beta r_{12}}/\beta r_{12} \qquad \text{if} \quad r_{12} \geqslant d, \\ &= 0 \qquad\qquad\qquad \text{if} \quad r_{12} < d. \end{aligned} \tag{2}$$

The parameter α in Eq. (1) is determined by the asymptotic form of t. For example, the Hamada–Johnston potential [3] has a one-pion exchange tail with $\alpha = 0.7067 \times 10^{13}\,\text{cm}^{-1}$.

For some applications, such as a microscopic description of elastic [4] and inelastic [5] scattering, it is necessary to have the expansion of t in multipoles of the individual nucleon coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$,

$$t(r_{12}) = 4\pi \sum_{L} t_L(r_1, r_2)\, Y_L{}^M(\hat{r}_1)\, Y_L^{M^*}(\hat{r}_2). \tag{3}$$

Multipoles may be required for values of L up to a few times 10. The various terms of Eq. (1) can be expanded in the same way.

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The multipole coefficients of $g(\beta r_{12})$ are then given by

$$g_L(\beta, r_1, r_2) = \frac{1}{2}\int_{-1}^{1} g(\beta r_{12})\, P_L(\mu)\, d\mu, \tag{4}$$

where $\mu = \cos\theta_{12}$. If $| r_1 - r_2 | \geqslant d$, then the $g_L(\beta, r_1, r_2) = g_L{}^Y(\beta, r_1, r_2)$, which are the multipole coefficients of an ordinary Yukawa interaction, and are given by the well-known expression

$$g_L{}^Y(\beta, r_1, r_2) = (\beta^2 r_1 r_2)^{-1/2}\, K_{L+1/2}(\beta r_>)\, I_{L+1/2}(\beta r_<), \tag{5}$$

where $r_>(r_<)$ is the greater (lesser) of r_1 and r_2. The $I_{L+1/2}$ and $K_{L+1/2}$ are modified spherical Bessel functions of the first and third kinds [6], respectively, and are generated by recurrence using the relations

$$\begin{aligned} K_{L+5/2}(x) &= K_{L+1/2}(x) + \frac{2L+3}{x} K_{L+3/2}(x), \\ I_{L+5/2}(x) &= I_{L+1/2}(x) - \frac{2L+3}{x} I_{L+3/2}(x). \end{aligned} \tag{6}$$

For the I a power series expansion is used for $x < 0.1$, downward recursion for $2x/L \leqslant 6$, and upward recursion for $2x/L > 6$, while upward recursion is used for the K for all x.

One of the advantages of fitting the effective interaction with a sum of cutoff Yukawa terms is now apparent. A typical elastic or inelastic scattering calculation might require $r_1, r_2 = 0, 0.1, 0.2,..., 15.0$ (in units of 10^{-13} cm); hence, $| r_1 - r_2 | = 0, 0.1, 0.2,..., 15.0$. For those values of $| r_1 - r_2 | > d \approx 1.0$, the $g_L(\beta, r_1, r_2)$ can be computed with the recurrence relations of Eq. (6). For given values of β, r_1, and r_2, this is a very fast way of obtaining the multipole coefficients for all values of L.

If $| r_1 - r_2 | < d$, then Eq. (4) can be written as

$$g_L(\beta, r_1, r_2) = g_L{}^Y(\beta, r_1, r_2) - \frac{1}{2}\int_{\gamma}^{1} \frac{e^{-\beta r_{12}}}{\beta r_{12}} P_L(\mu)\, d\mu, \tag{7}$$

where $\gamma = (r_1{}^2 + r_2{}^2 - d^2)/2r_1 r_2$. Using the expansion of $P_L(\mu)$ in powers of $(1 - \mu)$,

$$P_L(\mu) = \sum_{l=0}^{L} \frac{(-1)^l\,(L+l)!}{2^l (L-l)!\,(l!)^2} (1-\mu)^l, \tag{8}$$

enables one to write the g_L for the cutoff Yukawa as

$$g_L(\beta, r_1, r_2) = g_L{}^Y(\beta, r_1, r_2) - \frac{1}{\beta} \sum_{l=0}^{L} \frac{(-1)^l (L+l)!}{2^{2l+1}(L-l)!\,(l!)^2\,(r_1 r_2)^{l+1}}$$

$$\times \int_{|r_1-r_2|}^{d} e^{-\beta x}[x^2 - (r_1 - r_2)^2]^l\, dx \qquad \text{if} \quad |r_1 - r_2| < d,$$

$$= g_L{}^Y(\beta, r_1, r_2) \qquad \text{if} \quad |r_1 - r_2| \geqslant d. \tag{9}$$

The corresponding multipole coefficients t_L of the t matrix are then given by

$$t_L(r_1, r_2) = -V \sum_n A_n g_L(n\alpha, r_1, r_2). \tag{10}$$

The convenient feature of this algorithm is that the integrals in Eq. (10),

$$J_l(|r_1 - r_2|) = \int_{|r_1-r_2|}^{d} \sum_n A_n \frac{e^{-n\alpha x}}{n\alpha} [x^2 - (r_1 - r_2)^2]^l\, dx, \tag{11}$$

which must be computed extremely accurately for large L, do not depend on L and depend on r_1 and r_2 only in the combination $|r_1 - r_2| = 0, 0.1, 0.2,..., d \approx 1.0$, typically. A four-point Newton–Cotes integration formula with 800 mesh points was found to give sufficient accuracy for $L \lesssim 25$. These integrals are computed and stored as a function of $l = 0, 1,..., L_{\max}$ and $|r_1 - r_2|$ at the beginning of the calculation and used each time a new t_L is needed.

Several checks on the accuracy of this algorithm were made, one of which was the direct evaluation of Eq. (4) using Simpson's rule for various values of L, r_1, and r_2. For r_1 and r_2 near zero, the values of the g_L for $L \gtrsim 20$ are not given very accurately by the algorithm. However, for nucleon scattering at energies less than about 100 MeV, the high angular momentum partial waves are vanishingly small near the origin, so that inaccuracy in the g_L in this region will have no effect on the scattering cross sections. With this exception, the algorithm yields very good accuracy. Since the integrals J_l must be computed only once, the calculation of the g_L proceeds very quickly, requiring only slightly more computation time than the ordinary Yukawa interaction.

The subroutines for computing the multipole coefficients of a sum of up to six cutoff Yukawa terms ($n \leqslant 6$) using the method described above has been included in the FORTRAN code ATHENA-IV [7], which is used to calculate nuclear form factors for inealstic scattering. This code can be obtained upon request from the Argonne Code Center, Argonne National Laboratory.

This algorithm is useful for calculating the multipole coefficients of any effective interaction that can be fitted by a sum of cutoff Yukawa terms. For example, a very accurate fit to the long-range part of the even-state Hamada–Johnston potential [2] has been obtained using an unpublished routine written by R. Stafford. A sum of six terms was used in Eq. (1). The resulting coefficients A_n for the central interaction in singlet-even and triplet-even states and the second-order contribution from the tensor force to the interaction in triplet-even states are given in Ref. [7].

Another popular effective interaction is the long-range part of the Kallio–Kolltveit potential [8], the radial part of which has the form

$$\begin{aligned} g^{KK}(\alpha r_{12}) &= e^{-\alpha r_{12}} \qquad \text{if} \quad r_{12} \geqslant d, \\ &= 0 \qquad \text{if} \quad r_{12} < d. \end{aligned} \tag{12}$$

Since

$$e^{-\alpha r_{12}} = -\left(1 + \alpha \frac{d}{d\alpha}\right) e^{-\alpha r_{12}}/\alpha r_{12}, \tag{13}$$

we can use the central difference approximation for the derivative to write the multipole coefficients of g^{KK} in terms of three cutoff Yukawa terms,

$$\begin{aligned} &g_L^{KK}(\alpha, r_1, r_2) \\ &\quad = -g_L(\alpha, r_1, r_2) - \frac{\alpha}{2\Delta\alpha}\left[g_L(\alpha + \Delta\alpha, r_1, r_2) - g_L(\alpha - \Delta\alpha, r_1, r_2)\right], \end{aligned} \tag{14}$$

where the g_L are given by Eq. (9).

In conclusion, this technique of fitting the effective interaction with a sum of cutoff Yukawa terms and using the algorithm (9) to calculate the multipole coefficients of each term, constitutes a fast, accurate method of generating the multipole components of realistic interactions in nuclei.

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