THE BOUNDARY CONDITION PARAMETER IN R-MATRIX THEORY

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Abstract

In the general R-matrix theory of nuclear reactions, all measurable quantities such as the cross sections $\sigma_{cc'}$ should be independent of the choice of the boundary condition parameters B_c although the values of the level parameters E_λ and $\gamma_{\lambda c}$ depend on the B_c. For applications involving only a finite number of levels λ, it is not obvious that this is still the case as completeness arguments can no longer be used. It is shown here that $\sigma_{cc'}$ can be made independent of the choice of B_c for any finite number of levels and any number of channels, and the resulting formulae giving the dependence of E_λ and $\gamma_{\lambda c}$ on B_c are derived. An application is made to the pair of $5/2^-$ levels of ^{7}Li near 7 MeV excitation.

I. Introduction

In the R-matrix theory of nuclear reactions (Lane and Thomas 1958) the boundary condition parameters B_c do not play a very conspicuous role. In many applications their values have been chosen more or less arbitrarily. The reason for this is presumably that in the general theory, which involves infinite numbers of channels c and levels λ, all measurable quantities such as the cross sections $\sigma_{cc'}$ should be independent of the values of the B_c (and likewise of the values of the channel radii a_c). On the other hand, the corresponding values of the level parameters (the eigenenergies E_λ and reduced width amplitudes $\gamma_{\lambda c}$) depend on the values of the B_c (and a_c), as is evident from their definitions.

In applications of R-matrix theory, however, the general theory is approximated by assuming that only a finite number N_L of levels of given J^π contribute, and arguments based on completeness cannot be used. In this case, whether the number N_c of channels is finite or infinite, it is not obvious that the same values of $\sigma_{cc'}(E)$ can be obtained for any choice of the B_c (and it is not true for different choices of the a_c). A well-known case where it is possible is the one-level approximation with $\lambda = 1$, say, which requires γ_{1c} and $E_1 + \sum_c B_c \gamma_{1c}^2$ to be independent of B_c (Lane and Thomas 1958). It is also possible in the one-channel case with $c = a$, say, and formulae giving the dependence of E_λ and $\gamma_{\lambda a}$ on B_a have been given by Barker, Hay, and Treacy (1968) and used by Barker (1969, 1971).

In Section II it is shown that $\sigma_{cc'}(E)$ can be made independent of the B_c for general values of N_L and N_c, and explicit formulae are given for the resulting dependence of the E_λ and $\gamma_{\lambda c}$ on the B_c. These formulae have been used by Barker (1972). They are also applied in Section III, in the case $N_L = 2$, to the pair of $5/2^-$ levels of ^{7}Li near 7 MeV excitation, for which a peculiar behaviour of the $\gamma_{\lambda c}$ as functions of the B_c had previously been obtained (Spiger and Tombrello 1967).

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II. Dependence of Level Parameters on Boundary Condition Parameter

As far as possible, the notation of Lane and Thomas (1958) is used. From Lane and Thomas, the collision matrix $\mathbf{U}$ for given J^π can be written

$$\begin{aligned}\mathbf{U} &= \boldsymbol{\Omega}\mathscr{P}^{\frac{1}{2}}\{\mathbf{1}-\mathbf{R}(\mathbf{L}-\mathbf{B})\}^{-1}\{\mathbf{1}-\mathbf{R}(\mathscr{L}-\mathbf{B})\}\mathscr{P}^{-\frac{1}{2}}\boldsymbol{\Omega} \\ &= \boldsymbol{\Omega}\mathscr{P}^{\frac{1}{2}}\{(\mathbf{R}^{-1}+\mathbf{B})-\mathbf{L}\}^{-1}\{(\mathbf{R}^{-1}+\mathbf{B})-\mathscr{L}\}\mathscr{P}^{-\frac{1}{2}}\boldsymbol{\Omega}\,, \end{aligned} \tag{1}$$

where all matrices are in channel space; $\boldsymbol{\Omega}$, $\mathscr{P}$, $\mathbf{L}$, and $\mathscr{L}$ are external functions only; the matrix $\mathbf{R}$ has elements

$$R_{cc'} = \sum_\lambda \gamma_{\lambda c}\gamma_{\lambda c'}/(E_\lambda - E) \tag{2}$$

and in matrix notation is written

$$\mathbf{R} = \sum_\lambda \boldsymbol{\gamma}_\lambda \times \boldsymbol{\gamma}_\lambda/(E_\lambda - E)\,, \tag{3}$$

where it is assumed that λ runs from 1 to N_L; and $\mathbf{B}$ is the diagonal matrix with elements

$$B_{cc'} = B_c\,\delta_{cc'}\,.$$

From equation (1) it may be seen that $\mathbf{U}$ and therefore all cross sections are independent of $\mathbf{B}$ provided $\mathbf{R}^{-1}+\mathbf{B}$ is independent of $\mathbf{B}$.

Now, in terms of the E_λ, $\gamma_{\lambda c}$, and B_c, we wish to find values of the level parameters E'_λ and $\gamma'_{\lambda c}$ ($\lambda = 1, \ldots, N_L$) corresponding to the boundary condition parameters B'_c, such that

$$(\mathbf{R}')^{-1}+\mathbf{B}' = \mathbf{R}^{-1}+\mathbf{B} \tag{4}$$

for all values of E. For this purpose equation (4) is written in the form

$$\mathbf{R}' = \{\mathbf{1}-\mathbf{R}(\mathbf{B}'-\mathbf{B})\}^{-1}\mathbf{R}$$

and it is assumed (c.f. Chapter IX of Lane and Thomas 1958) that quantities $A_{\mu\nu}$ exist such that

$$\mathbf{R}' = \sum_{\mu\nu} (\boldsymbol{\gamma}_\mu \times \boldsymbol{\gamma}_\nu) A_{\mu\nu}\,, \tag{5}$$

requiring

$$\mathbf{R} = \{\mathbf{1}-\mathbf{R}(\mathbf{B}'-\mathbf{B})\}\sum_{\mu\nu} (\boldsymbol{\gamma}_\mu \times \boldsymbol{\gamma}_\nu) A_{\mu\nu}\,. \tag{6}$$

We can now substitute the expression (3) for $\mathbf{R}$ into equation (6) and then use the fact that $\mathbf{B}'-\mathbf{B}$ is diagonal to write

$$(\boldsymbol{\gamma}_\lambda \times \boldsymbol{\gamma}_\lambda)(\mathbf{B}'-\mathbf{B})(\boldsymbol{\gamma}_\mu \times \boldsymbol{\gamma}_\nu) = (\boldsymbol{\gamma}_\lambda \times \boldsymbol{\gamma}_\nu)\xi_{\lambda\mu}\,,$$

where

$$\xi_{\lambda\mu} = \sum_c (B'_c - B_c)\gamma_{\lambda c}\gamma_{\mu c}\,.$$

This gives

$$\sum_{\lambda\nu} (\boldsymbol{\gamma}_\lambda \times \boldsymbol{\gamma}_\nu)\left(-\delta_{\lambda\nu}/(E_\lambda - E) + A_{\lambda\nu} - \sum_\mu \xi_{\lambda\mu} A_{\mu\nu}/(E_\lambda - E)\right) = 0\,,$$

which is satisfied if, for all λ, ν (from 1 to N_L),

$$(E_\lambda - E)A_{\lambda\nu} - \sum_\mu \xi_{\lambda\mu} A_{\mu\nu} = \delta_{\lambda\nu}, \tag{7}$$

and these are the equations for determining the $A_{\lambda\nu}$.

Consider now a change of notation (for this paragraph only) in which matrix notation is used for matrices in level space and the channel labels are written explicitly. In this case the $A_{\lambda\nu}$ are the elements of an $N_L \times N_L$ matrix **A**, and equations (7) can be written

$$\mathbf{A} = (\mathbf{C} - E\mathbf{1})^{-1}, \tag{8}$$

where **C** has elements

$$C_{\lambda\mu} = E_\lambda \delta_{\lambda\mu} - \sum_c (B'_c - B_c)\gamma_{\lambda c}\gamma_{\mu c}, \tag{9}$$

while (5) can be written

$$R'_{cc'} = \tilde{\gamma}_c \mathbf{A} \gamma_{c'}, \tag{10}$$

where γ_c is a single-column matrix with elements $\gamma_{\lambda c}$. Expressions for the level parameters occurring in $R'_{cc'}$ are now obtained by reducing **C**, and therefore **A**, to diagonal form. This may be accomplished by means of a transformation using an orthogonal matrix **K**, since **C** is real and symmetric, i.e.

$$\mathbf{K}\mathbf{C}\tilde{\mathbf{K}} = \mathbf{D}, \tag{11}$$

where

$$D_{\lambda\mu} = D_\lambda \delta_{\lambda\mu}.$$

The D_λ are the eigenvalues of the matrix **C** and, for given λ, the $K_{\lambda\mu}$ are the elements of the normalized eigenvector corresponding to D_λ. Introduction of equations (8) and (11) into (10) with

$$\mathbf{K}\tilde{\mathbf{K}} = \tilde{\mathbf{K}}\mathbf{K} = \mathbf{1} \tag{12}$$

gives

$$R'_{cc'} = \tilde{\gamma}_c \tilde{\mathbf{K}} (\mathbf{D} - E\mathbf{1})^{-1} \mathbf{K} \gamma_{c'},$$

which is of the required form

$$R'_{cc'} = \sum_\lambda \gamma'_{\lambda c}\gamma'_{\lambda c'}/(E'_\lambda - E)$$

provided

$$E'_\lambda = D_\lambda \qquad \text{and} \qquad \gamma'_c = \mathbf{K}\gamma_c. \tag{13a, b}$$

This demonstrates the possibility of making $\sigma_{cc'}(E)$ independent of B_c and gives the relations between the level parameters necessary for this. The essential task involved is the standard one of diagonalizing the matrix **C** defined by (9); then the E'_λ are its eigenvalues and the $\gamma'_{\lambda c}$ are given in terms of its eigenvectors by (13b).

Similar considerations apply to a reaction in which the system with levels λ is formed as a product nucleus that then decays. In this case a form for the cross section has been proposed (Barker 1967) in which the dependence on B_c is contained in the

term

$$\{\mathbf{1}-\mathbf{R}(\mathbf{L}-\mathbf{B})\}^{-1}\,\mathbf{Q}\,, \tag{14}$$

where

$$\mathbf{Q} = \sum_{\lambda} \gamma_{\lambda} \times \mathbf{g}_{\lambda}/(E_{\lambda}-E)\,, \tag{15}$$

$\mathbf{g}_{\lambda}$ being a single-column matrix in the space of formation channels x with the feeding amplitudes $g_{\lambda x}$ as elements. Since the term (14) can be written as

$$\{(\mathbf{R}^{-1}+\mathbf{B})-\mathbf{L}\}^{-1}\,\mathbf{R}^{-1}\,\mathbf{Q}$$

and $\mathbf{R}^{-1}+\mathbf{B}$ is independent of $\mathbf{B}$, it is necessary that $\mathbf{R}^{-1}\,\mathbf{Q}$ be independent of $\mathbf{B}$, that is,

$$(\mathbf{R}')^{-1}\,\mathbf{Q}' = \mathbf{R}^{-1}\,\mathbf{Q} \qquad \text{or} \qquad \mathbf{Q}' = \mathbf{R}'\mathbf{R}^{-1}\,\mathbf{Q} = \{\mathbf{1}-\mathbf{R}(\mathbf{B}'-\mathbf{B})\}^{-1}\,\mathbf{Q}\,.$$

By the same method as before, it follows that

$$\mathbf{Q}' = \sum_{\mu\nu} (\gamma_{\mu} \times \mathbf{g}_{\nu}) A_{\mu\nu}\,,$$

thus leading to the relation between matrices in level space

$$\mathbf{g}'_{x} = \mathbf{K}\mathbf{g}_{x}\,. \tag{16}$$

From equations (13b), (16), and (12), it follows that

$$\sum_{\lambda} \gamma_{\lambda c}\gamma_{\lambda c'} \qquad \text{and} \qquad \sum_{\lambda} g_{\lambda x} g_{\lambda x'}$$

are independent of B_c for all c, c', x, and x'.

III. $5/2^-$ Levels of ^{7}Li

Spiger and Tombrello (1967) (hereinafter referred to as ST) extracted complex phase shifts for ^{3}H+α scattering from their measurements of ^{3}H(α,α)^{3}H, ^{3}H(α,n)^{6}Li, and ^{3}H(α,n')^{6}Li*. The $f_{5/2}$ phase shift indicated $5/2^-$ levels of ^{7}Li at about 6·6 and 7·5 MeV. ST used the two-level, two-channel R-matrix formulae to fit this phase shift. They investigated numerically the variation of the level parameters with change of boundary condition parameters, and found their results rather disturbing, in that one of the reduced width amplitudes varied by a factor of more than five over a small range of B_c values. This variation is now studied on the basis of the analytical formulae of the preceding section.

The two levels in the R-matrix formulae are labelled by $\lambda = 1$ and 2 with $E_1 \leqslant E_2$, while the two channels ^{3}H+α (f-wave) and ^{6}Li+n (p-wave) are labelled by $c = \alpha$ and n (equivalent to e and r in ST). For the particular case $B_{\alpha} = -3$ and $B_{\mathrm{n}} = -1$, ST gave values of the $\gamma^2_{\lambda c}$. We use their best values and, without loss of generality, assume all $\gamma_{\lambda c} \geqslant 0$. Also ST gave values of the resonance energies E_{res} rather than of E_{λ}. We assume that values of E_{λ} may be obtained with sufficient

accuracy by taking for each level

$$E_\lambda = E_{\rm res} + \sum_c \gamma_{\lambda c}^2 \{S_c(E_{\rm res}) - B_c\}, \tag{17}$$

where S_c is the shift factor, which may be calculated. The level parameters for the $5/2^-$ levels of ^{7}Li obtained in this way are (for $B_\alpha = -3$ and $B_{\rm n} = -1$):

λ	$E_{\rm res}$ (MeV)	E_λ (MeV)	$\gamma_{\lambda\alpha}$ (MeV$^{\frac{1}{2}}$)	$\gamma_{\lambda{\rm n}}$ (MeV$^{\frac{1}{2}}$)
1	7·47	7·65	0·155	1·095
2	6·64	10·20	1·761	0·0

The inversion of the E_λ values relative to the $E_{\rm res}$ values may be noted. This is due to the fact that B_α differs appreciably from S_α over the energy range concerned while the $\gamma_{\lambda\alpha}$ values of the two levels are very different. ST distinguished the two levels as lower or upper (based on $E_{\rm res}$ values), or used spectroscopic notation (^{2}F$_{5/2}$ or ^{4}P$_{5/2}$) based on the reduced widths of the levels, but either nomenclature can lead to confusion when the boundary condition parameters are varied.

From the parameter values given above and the formulae (13) of Section II, values of E_λ and $\gamma_{\lambda c}$ may be calculated for other values of B_c such that exactly the same fit is obtained to the f$_{5/2}$ phase shift. Figure 1(*a*) shows the resulting dependence of E_λ and $\gamma_{\lambda c}$ on B_α for three fixed values of $B_{\rm n}$, while Figure 1(*b*) shows the dependence on $B_{\rm n}$ for fixed B_α.

The graphs of Figure 1 illustrate some of the results obtained by ST. They found that changing $B_{\rm n}$ did not affect $\gamma_{\lambda\alpha}$, but it is seen that this is true only for $B_\alpha = -3$ (as used by ST) because $\gamma_{2{\rm n}} \equiv 0$ for this value of B_α. Figure 19 of ST shows the dependence on B_α that they found for $\gamma_{\lambda\alpha}$ (or rather for γ_e, which they describe as the α-particle reduced width amplitude of the upper level, or the ^{4}P$_{5/2}$ state). Their figure corresponds to part of the right-hand panel of Figure 1(*a*), in which the range of B_α values for which ST were able to find a solution is indicated by the arrows. It is seen that their γ_e corresponds in one part of the range to $\gamma_{1\alpha}$ and in the other part to $\gamma_{2\alpha}$. The correspondence is not exact as it seems that ST did not allow a dependence of $\gamma_{\lambda{\rm n}}$ on B_α and hence could not find a good fit in the region where $\gamma_{\lambda{\rm n}}$ is varying rapidly.

We now consider the values of the E_λ and $\gamma_{\lambda c}$ that should be fitted in a shell-model calculation of the levels of ^{7}Li. Usually such calculations include states of only the lowest shell-model configuration $(1s)^4(1p)^3$ so that the shell-model eigenfunctions satisfy the same boundary condition at the channel surface as do the eigenstates in the internal region in *R*-matrix theory. Consequently the energies in the shell-model calculation should be taken as the *R*-matrix eigenenergies E_λ, all for the same values of B_c rather than, say, the resonance energies.* Differences between the shell-model energies are probably more reliable than their absolute values. Also ratios of reduced width amplitudes for different levels but the same channel, say γ_{2c}/γ_{1c}, can be calculated from the shell-model wavefunctions without specifying the shape of the single-particle radial wavefunctions. Since the energy difference

* In Barker (1971), shell-model states of different configurations were involved and it was appropriate to choose different B_c values when determining the properties of the different states.

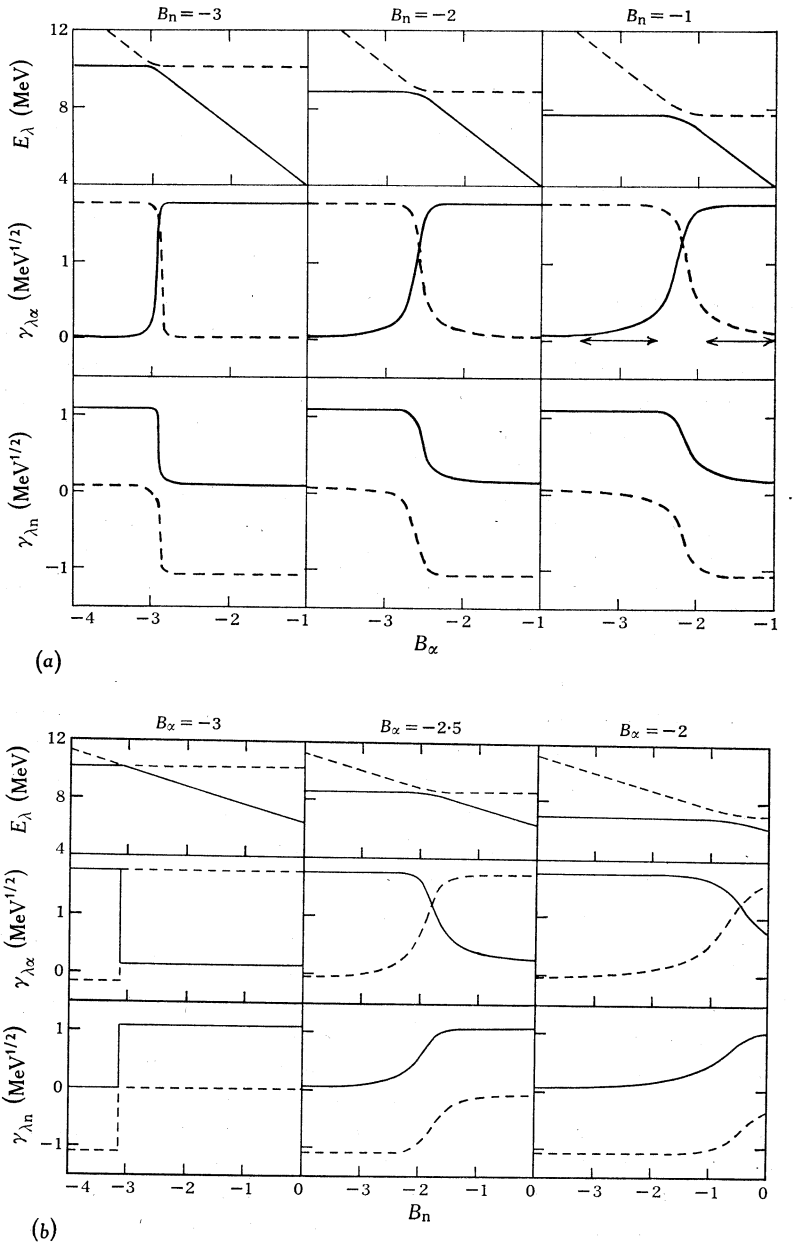

Fig. 1.—Dependence of the level parameters E_λ and $\gamma_{\lambda c}$ on the boundary condition parameters B_c required to give the same values of the $f_{5/2}$ phase shift in $^3H+\alpha$ scattering: (*a*) dependence on B_α for three values of B_n; (*b*) dependence on B_n for three values of B_α. The solid curves refer to $\lambda = 1$, the dashed curves to $\lambda = 2$.

E_2-E_1 and the ratios γ_{2c}/γ_{1c} depend sensitively on the B_c, it is necessary to specify the most appropriate values of the B_c. One expects the best agreement between the shell-model states and the *R*-matrix internal eigenstates when each B_c is set equal to a mean value of the shift factor S_c in the energy range of interest (see Appendix III of Barker, Hay, and Treacy 1968). In the present case at excitation energies of 6·64 and 7·47 MeV in ^{7}Li, the values of S_α are −1·85 and −1·61 and of S_n −1·25 and −0·88 respectively (for channel radii $a_\alpha = a_n = 4{\cdot}0$ fm, as used by ST).

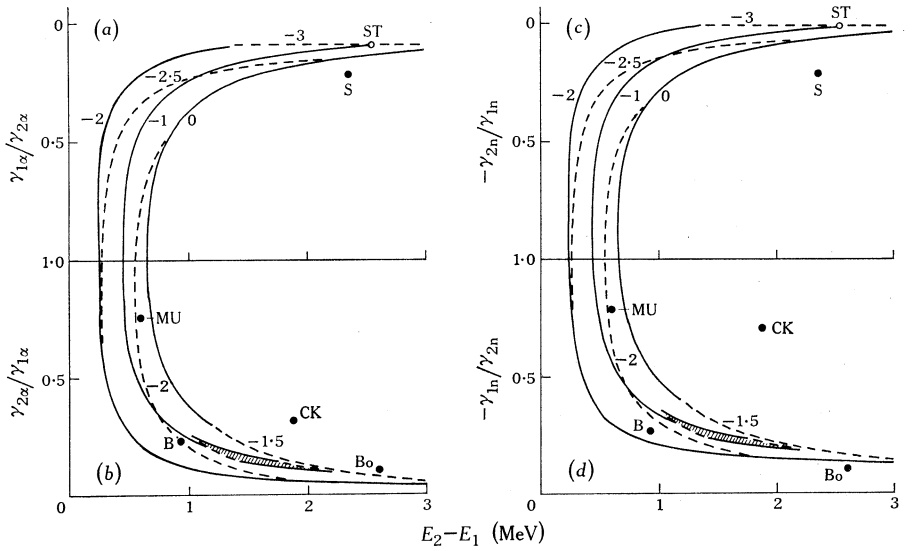

Fig. 2.—Ratios of α-particle and neutron reduced width amplitudes as functions of eigenenergy separation. The curves come from the requirement of the same values of the $f_{5/2}$ phase shift in $^3H+\alpha$ scattering, and are for the indicated fixed values of the boundary condition parameters B_α (dashed curves) and B_n (solid curves). The regions in which the B_c are close to the corresponding shift factors are shown hatched. The open circles mark the original parameter values of ST, while the other points show the values obtained from shell-model calculations by: MU, Meshkov and Ufford (1956); S, Soper (1957); Bo, Boyarkina (1964); CK, Cohen and Kurath (1965); B, Barker (1966).

Figure 2 shows the dependences of E_2-E_1 and the γ_{2c}/γ_{1c} on the B_c in a more convenient form than Figure 1 by giving in (*b*) and (*d*) $\gamma_{2\alpha}/\gamma_{1\alpha}$ and $-\gamma_{1n}/\gamma_{2n}$ as functions of E_2-E_1 for constant values of B_α and of B_n; Figures 2(*a*) and 2(*c*) give the inverse ratios. The hatched regions are bounded by the curves $B_\alpha = -1{\cdot}85$ and $-1{\cdot}61$ and $B_n = -1{\cdot}25$ and $-0{\cdot}88$. In these regions the 6·64 MeV resonance is due mainly to level 1 and the 7·47 MeV resonance to level 2, and, as $\gamma_{2\alpha}/\gamma_{1\alpha}$ and $|\gamma_{1n}/\gamma_{2n}|$ are both small, more weight should be attached to values of B_α near −1·85 and of B_n near −0·88, i.e. to the upper left-hand corners of the hatched areas. Thus in shell-model calculations one should try to fit values of E_2-E_1 and γ_{2c}/γ_{1c} in the hatched areas, and preferably near their left-hand ends. It may be noted that the parameter values given by ST (open circles in Figs. 2(*a*) and (2*c*)) are not suitable for direct comparison with shell-model calculations, as they lie far from the hatched areas. Other points marked in Figure 2 give results from some

published shell-model calculations. It is seen that several of these, in particular those of Soper (1957), lie far from the hatched areas.

Although only the $5/2^-$ levels of ^{7}Li have been discussed in this section, similar considerations apply to the $5/2^-$ levels of ^{7}Be. The present example has been used to illustrate the general result that, when R-matrix theory is used to fit experimental data, it is not necessary to treat the boundary condition parameters B_c as adjustable, since any fit to the data with a particular set of B_c values can be duplicated exactly for any other set of B_c values. If, however, the values of the level parameters E_λ and $\gamma_{\lambda c}$ obtained from such a fit are to be compared with values calculated from some nuclear model, they should be chosen to correspond to the most appropriate values of B_c.

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