Relation between the optical model and the valence model of $E1$ neutron capture at and between resonances

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We show that there are simple relations between the valence model of neutron capture and the optical model. These are derived without recourse to any particular formal framework. The relations show that the predictions of the valence capture model involve the full optical potential and that it is inadequate to use the real part alone.

Recently the valence model of neutron capture has been discussed[1-3] within the framework of the shell-model theory of nuclear reactions. This study presented estimates for experimental quantities like background (inter-resonance) capture, suggesting that it is reasonably accurate in practice to obtain these from the real part of the optical potential (see Fig. 1 of Ref. 2 and Sec. 3 of Ref. 3). In a study[4] in 1960, the full potential was used. In this note, we see that it is unnecessary to air these matters within a particular framework (such as the shell-model or R-matrix theory of reactions). Instead one can, from a few simple equations, derive all interesting quantities for capture, and settle the issue about the optical potential.

For simplicity we will confine the discussion to incident s waves and spinless particles. These restrictions are readily removed. The neutron capture cross section at energy E to a final state f is

$$\sigma_{nf}(E) = \pi k^2 \,|\, S_{nf}(E) \,|\,^2 , \tag{1}$$

where k is the incident wave number $mv/\hbar_0$. The quantity S_{nf} may be expressed in terms of reactance matrix elements

$$S_{nf}(E) = -2i\,K_{nf}(E)\,[1 - i\,K_{nn}(E)]^{-1} . \tag{2}$$

K_{nn} is related to the elastic scattering phase shift δ:

$$K_{nn} = \tan\delta , \tag{3}$$

and K_{nf} may be written as the $E1$ matrix element

$$K_{nf} = \langle f \,|\, D \,|\, \psi_E \rangle , \tag{4}$$

where ψ_E is the elastic scattering standing-wave solution with asymptotic form

$$\psi_E \to \frac{1}{r(\hbar v)^{1/2}} [\sin(kr) + K_{nn}\cos(kr)]\phi_0 . \tag{5}$$

ϕ_0 is the target state. All unimportant factors are absorbed into the operator D. For all quantities S_{nf}, K_{nf}, K_{nn}, a bar indicates that E is replaced by $E + i\epsilon$ where $\epsilon \gg$ level spacing. The average value of S_{nf} is:

$$\bar{S}_{nf} = -2i\,\bar{K}_{nf}(1 - i\,\bar{K}_{nn})^{-1} . \tag{6}$$

K_{nn} may be divided into local levels plus a background of distant levels which may be identified with $\mathrm{Re}\bar{K}_{nn}$; similarly with K_{nf}. Ignoring the local levels in K_{nn}, K_{nf} in (2) leads to a quantity that we can call the background capture amplitude:

$$S_{nf}(\mathrm{back}) = \frac{-2i\,\mathrm{Re}\bar{K}_{nf}}{1 - i\,\mathrm{Re}\bar{K}_{nn}} . \tag{7}$$

For a single level λ and no background

$$\begin{aligned} K_{nn} &= \tfrac{1}{2}\Gamma_{\lambda n}(E_\lambda - E)^{-1} , \\ K_{nf} &= \tfrac{1}{2}(\Gamma_{\lambda n}\Gamma_{\lambda f})^{1/2}(E_\lambda - E)^{-1} . \end{aligned} \tag{8}$$

When both the background and a single level are present, we get, on adding background terms to (8) and inserting in (2):

$$\begin{aligned} S_{nf} &= -i\,\frac{(\Gamma_{\lambda n}\Gamma_{\lambda f})^{1/2} + 2(E_\lambda - E)(\mathrm{Re}\bar{K}_{nf})}{(E_\lambda - E)(1 - i\,\mathrm{Re}\bar{K}_{nn}) - \frac{1}{2}i\,\Gamma_{\lambda n}} \\ &= e^{i\phi}\left(|\, S_{nf}(\mathrm{back}) \,| + \frac{(\tilde{\Gamma}_{\lambda n}\tilde{\Gamma}_{\lambda f})^{1/2} e^{-i\beta}}{\tilde{E}_\lambda - E - \frac{1}{2}i\,\tilde{\Gamma}_{\lambda n}} \right) . \end{aligned} \tag{9}$$

The last expression results from rearrangement of the first one. We give explicit form only to the relative phase β since there has been interest in this[1,3,5,6].

$$\cot\beta = \mathrm{Re}\bar{K}_{nn} - \left(\frac{\Gamma_{\lambda f}}{\Gamma_{\lambda n}}\right)^{1/2} \frac{1 + (\mathrm{Re}\bar{K}_{nn})^2}{\mathrm{Re}\bar{K}_{nf}} . \tag{10}$$

The imaginary parts of $\bar{K}_{nn}, \bar{K}_{nf}$ determine the

average residues:

$$2\pi \operatorname{Im}\bar{K}_{nn}=\langle\Gamma_{\lambda n}\rangle\rho\,, \tag{11}$$

$$2\pi \operatorname{Im}\bar{K}_{nf}=\langle(\Gamma_{\lambda n}\Gamma_{\lambda f})^{1/2}\rangle\rho\,, \tag{12}$$

where ρ is level density.

We identify the valence model[7,8] contribution to capture as that from the entrance channel components in the initial and final states. Defining

$$\begin{aligned} u_E(r)&\equiv\langle\phi_0\,|\,\psi_E\rangle\,,\\ u_f(r)&\equiv\langle\phi_0\,|f\rangle\,, \end{aligned} \tag{13}$$

the model expression for K_{nf} is, from (4):

$$K_{nf}=\langle u_f\,|\,D\,|\,u_E\rangle\,; \tag{14}$$

then

$$\bar{K}_{nf}=\langle u_f\,|\,D\,|\,u_E(\text{opt})\rangle\,, \tag{15}$$

where $u_E(\text{opt})$ is the optical model solution. By definition this equals $u_{(E+i\epsilon)}=\bar{u}$. Similarly

$$\bar{K}_{nn}=\tan\delta(\text{opt})\,, \tag{16}$$

where $\delta(\text{opt})$ is the optical model phase shift. Equations (15) and (16) give $\bar{K}_{nf}$ and $\bar{K}_{nn}$ in terms of the optical model. From (7) and (11), (12) we get similar expressions for other quantities:

$$S_{nf}(\text{back})=-2i\,\frac{\operatorname{Re}\langle u_f\,|\,D\,|\,u_E(\text{opt})\rangle}{1-i\operatorname{Re}\tan\delta(\text{opt})}\,, \tag{17}$$

$$\left(\frac{\Gamma_{\lambda f}}{\Gamma_{\lambda n}}\right)^{1/2}=\frac{\operatorname{Im}\langle u_f\,|\,D\,|\,u_E(\text{opt})}{\operatorname{Im}\tan\delta(\text{opt})}, \tag{18}$$

where for (18) we have assumed $\langle\Gamma_{\lambda f}{}^{1/2}\Gamma_{\lambda n}{}^{1/2}\rangle=\langle\Gamma_{\lambda f}\rangle^{1/2}\langle\Gamma_{\lambda n}\rangle^{1/2}$. These agree, in the low-energy limit, with the expressions used in the early study[4] of capture, but disagree with those used recently.[1-3] Equation (18) is equivalent to (85) of Ref. 4 when specialized to low energy.

Suppose that the optical model solution $u_E(\text{opt})$ is dominated over an appreciable energy range by a single giant resonance, say $u_0(r)$ with $d(u_0r)/dr=0$ at $r=a$, a being the nuclear radius. For $r<a$, we have:

$$u_E(\text{opt})=\frac{\frac{1}{2}\sec(ka)\,(\Gamma_{0n})^{1/2}}{E_0-E-iW_0}u_0(r)\,, \tag{19}$$

while, for $r>a$:

$$u_E(\text{opt})=\frac{1}{r(\hbar v)^{1/2}}\left(\sin[k(r-a)]\sec(ka)+\frac{\frac{1}{2}(\Gamma_{0n})\sec^2(ka)}{E_0-E-iW_0}\cos(kr)\right). \tag{20}$$

$u_0(r)$ is normalized inside $r=a$:

$$\int_0^a|u_0|^2r^2dr=1\,. \tag{21}$$

Γ_{0n}, $2W_0$ are the natural decay and broadening widths of the giant resonance. Using (19), (20) in (15):

$$\bar{K}_{nf}=\frac{1}{(\hbar v)^{1/2}}\sec(ka)\left\langle u_f\,|\,\tilde{D}\,|\,\frac{\sin[k(r-a)]}{r}\right\rangle+\frac{\frac{1}{2}\sec(ka)(\Gamma_{0n}\Gamma_{0f})^{1/2}}{E_0-E-iW_0}, \tag{22}$$

where

$$\Gamma_{0f}{}^{1/2}=\langle u_f\,|\,D\,|\,\tilde{u}_0\rangle\,. \tag{23}$$

$\tilde{u}_0$ is u_0 for $r<a$; for $r>a$, $\tilde{u}_0$ is continued as a cosine:

$$\tilde{u}_0(r>a)=u_0(a)\frac{\cos(kr)}{\cos(ka)}\,. \tag{24}$$

The quantity $\tilde{D}$ is D for $r>a$ and zero for $r<a$. Near the dominant giant resonance, the optical model phase shift is given by:

$$\bar{K}_{nn}=\tan\delta(\text{opt})=-\tan(ka)+\frac{\frac{1}{2}\Gamma_{0n}\sec^2(ka)}{E_0-E-iW_0}\,. \tag{25}$$

From (18), (22), (25), noting that $\langle\Gamma_{\lambda f}{}^{1/2}\Gamma_{\lambda n}{}^{1/2}\rangle=\langle\Gamma_{\lambda f}\rangle^{1/2}\langle\Gamma_{\lambda n}\rangle^{1/2}$ exactly in the present special situation:

$$\left(\frac{\Gamma_{\lambda f}}{\Gamma_{\lambda n}}\right)^{1/2}=\left(\frac{\Gamma_{0f}}{\Gamma_{0n}}\right)^{1/2}\cos(ka)\,. \tag{26}$$

Insertion of this into (10), along with (22), (25), gives:

$$\cot\beta=\tan(ka)-\left(\frac{\frac{1}{2}\Gamma_{0n}(E_0-E)}{(E_0-E)^2+W_0{}^2}\right)^{-1}, \tag{27}$$

if the external ($\tilde{D}$) term in (22) is neglected. $S_{nf}(\text{back})$ is obtained from (7), (22), (25). When $ka\ll1$, it is:

$$S_{nf}(\text{back})=-2i\left[\left(\frac{mk}{\hbar^2}\right)^{1/2}\left\langle u_f\,|\,\tilde{D}\,|\,\frac{(r-a)}{r}\right\rangle+\frac{(\Gamma_{0n}\Gamma_{0f})^{1/2}(E_0-E)}{(E_0-E)^2+W_0{}^2}\right]. \tag{28}$$

Without resorting to any special framework of formal theory, we have derived in a simple way expressions for interesting quantities characterizing capture. This has been done generally [Eqs. (6)–(12)] and for the valence model [Eqs. (15)–(18)]. It is clear that the background capture amplitude (17) involves the real part of the optical model quantities, not quantities from the real part of the optical potential. This is of crucial importance. From (27) and (28) we see that, near $E_0\approx E$, the latter view leads to the large values for $\tan\beta$ and $S_{nf}(\text{back})$ that have been given in recent publications.[1-3] The values of $S_{nf}(\text{back})$ are in sharp contrast to the small values near $E_0\approx E$ reported in earlier calculations[4] which used the optical potential. We disagree with the assertion in Ref. 3,

Sec. 3 that the contribution of distant resonance terms (i.e., background capture) can be accurately estimated from a real potential (as depicted in Fig. 1 of Ref. 2). This is true only for less interesting situations (those with no nearby single particle state). This difference in calculational recipe between Refs. 3 and 4 can be traced partly to a difference in physical interpretation. Ref. 3 suggests that one should not use a complex potential for situations in which no resonance average is taken. This novel view is in conflict not only with Ref. 4 but also with the original study[9] on the optical potential in which zero-energy scattering is fitted. In our view, the complex potential can and should be used.

Finally, we comment on the evaluation of (26) for low energies where $\cos(ka) \approx 1$. In the studies[10] of p-wave neutron capture in ^{98}Mo and ^{96}Zr, Γ_{0n} was evaluated with the single-particle reduced width $3\hbar^2/2ma^2$, whereas Γ_{0f} was taken from the published values[7] of $E1$ matrix elements involving an initial state u_0 bound by an energy of the order of 100 keV and normalized over all space. One now sees that both Γ_{0n} and Γ_{0f} should be increased: Γ_{0n} because the Woods-Saxon values of the reduced width are larger than $3\hbar^2/2ma^2$, and Γ_{0f} because the correct quantity should have u_0 normalized over the interior only. For a Woods-Saxon potential with a diffuseness parameter 0.69, the single-particle reduced width[11] is $4.2\hbar^2/ma^2$. Numerical calculations of Γ_{0f} using a Woods-Saxon potential[12] have been carried out for $s \to p$ and $p \to s$ transitions in the $3s$ and $3p$ giant resonances, respectively. (Note that, for general l wave the $\cos\rho$ function in (24) is replaced by the irregular Bessel function $\rho j_{-l}(\rho)$ with $\rho = kr$ or ka.) When the normalization of u_0 is carried out over the interior region, the results show that Γ_{0f} is 1.5 to 5.0 times larger than previous estimates.[8] As a result, the two corrections for Γ_{0n} and Γ_{0f} are comparable and cancel each other.

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