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# Electron capture and nuclear resonances

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**Abstract.** We show that the simple two-amplitude Blair-Anholt formula for ionization in the presence of a nuclear resonance can be generalized to electron capture. This generalization has been obtained from a fully quantum mechanical treatment by performing approximations which are the large-angle counterpart of those used to obtain the standard semiclassical $t$ matrix for forward scattering. The resulting formula involves electronic amplitudes which must be calculated for a prescribed broken straight line nuclear trajectory. Application of this simple two-amplitude formula to different systems shows that it is able to describe the gross features of the electron capture across a nuclear resonance.

## 1. Introduction

Over the past few years considerable effort has been directed towards experimental investigations of the energy dependence of electron capture across a nuclear resonance (Horsdal-Pedersen *et al* 1982, 1987, Scheurer *et al* 1985, Horsdal *et al* 1986, Baker *et al* 1987, 1988). This effort has been motivated by the fact that the usual criterion for a manifest interference between an elastic scattering resonance and an atomic process (i.e. that $\Delta E \simeq \Gamma$, where $\Delta E$ is the atomic energy transfer and $\Gamma$ the nuclear width) is more favourable to electron capture than to total ionization. For this last process, which has been extensively studied (see Meyerhof *et al* 1985 for a review on the subject), the interference structure is smeared out by the energy spread of the emitted electrons. Moreover, the nuclear resonances that can be studied are restricted by the fact that the transfer energy (i.e. the ionization energy) is often almost too small to verify the above criterion for interference phenomena (Amundsen and Jakubassa-Amundsen 1984a). From the theoretical point of view, the interplay of nuclear and atomic physics is of great interest because it gives additional information on the atomic amplitudes: the relative phases and magnitudes of the capture amplitudes which describe the various electron-capture-nuclear-resonance sequences are now accessible to experimental test. Unfortunately, the theoretical work on the subject is limited and, up until now, experimental data have been only confronted with the predictions of the large-angle strong potential Born (SPB) approximation developed by Amundsen and Jakubassa-Amundsen (1984a) and Jakubassa-Amundsen and Amundsen (1985). The SPB model leads to a three-amplitudes formula which describes the sequences *etf*, *eft* and *fet*, where *e*, *t*, and *f* denote virtual excitation of the target, electron capture and nuclear scattering, respectively. The gross features of the interference phenomena are well reproduced by the SPB calculation.

The interplay between atomic and nuclear processes must be studied at large angles, where the resonant scattering is not clouded by the Coulomb dispersion. From a

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semiclassical point of view, these large-angle collisions only involve small impact parameters, and so the nuclear path can be described by a broken straight line. This simplification of the full quantum problem has been successfully applied in the calculation of large-angle capture probabilities in the absence of nuclear resonances (Kocbach and Briggs 1984, Amundsen and Jakubassa-Amundsen 1984b, Maidagan and Salin 1987, Maidagan 1988). It is interesting to extend this semiclassical view to electron-capture processes in the presence of nuclear resonances. The aim of the present paper is to show that this generalization can be obtained from the full quantum formulation by performing approximations which can be seen as the large angle counterpart of those used to obtain the standard semiclassical $t$ matrix for forward scattering (Wilets and Wallace 1968, Bransden and Coleman 1972, Flannery and McCann 1973). We obtain a very simple two-amplitude formula which describes the sequence *ef* and *fe* by means of semiclassical charge exchange semi-amplitudes which must be calculated for a prescribed broken straight line nuclear trajectory. This two-amplitude formula is also valid for ionization and is closely related to the pioneering Blair–Anholt expression (Blair and Anholt 1982). Our second aim is to apply the above formulation in order to present an additional numerical reference by calculating approximate exchange probabilities for all the systems which have been the subjects of experimental study. In this application the approximate semi-amplitudes are calculated by using the broken straight line version of the peaking impulse approximation (PIA). We compare our theoretical results with the SPB ones and with experimental data for protons on $^{12}C$, $^{14}N$, $^{20}Ne$ and $^{22}Ne$. Atomic units are used throughout unless otherwise indicated.

## 2. The quantum amplitude

We shall consider the capture of an electron of a heavy atom by a light bare projectile. An independent electron model for the multi-electronic target will be assumed and therefore we are concerned with a three-body system as a simple model for the charge exchange process. The coordinates $\boldsymbol{R}$, $\boldsymbol{R}_i$, $\boldsymbol{R}_f$, $\boldsymbol{r}_T$ and $\boldsymbol{r}_P$ are displayed in figure 1. In order to take into account exactly the strong $\boldsymbol{R}$ dependent internuclear interaction it is advantageous to work with coordinates $\boldsymbol{R}$ and $\boldsymbol{r}_T$ (we are interested here in close

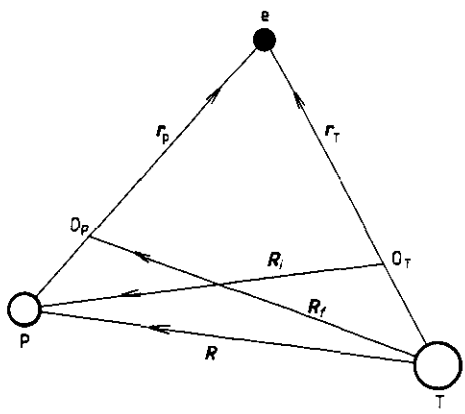


**Figure 1.** Coordinates for the three-body problem. $O_T$ and $O_P$ denote the centre of mass of target-electron and projectile-electron systems, respectively.

encounter collisions for which the internuclear potential cannot be treated perturbatively). For this choice the total Hamiltonian reads

$$H = H_N + H_T + V_P + V_R \tag{1}$$

where $H_N$ is the nuclear Hamiltonian which describes the internuclear motion, $H_T$ is the electronic Hamiltonian in the target field, $V_P$ denotes the projectile-electron potential and $V_R$ reflects the fact that $(\boldsymbol{R}, \boldsymbol{r}_T)$ are not Jacobi coordinates for the three-body problem. It is the so-called target recoil potential and it reads

$$V_R = M_T^{-1}\mathbb{P} \cdot \boldsymbol{p} = -i\Lambda M_T^{-1}[\boldsymbol{R}, H_N] \cdot \boldsymbol{p} \tag{2}$$

where $\boldsymbol{p}$ and $\mathbb{P}$ are the conjugate momenta of $\boldsymbol{r}_T$ and $\boldsymbol{R}$, respectively, $\Lambda$ is the nuclear reduced mass and $M_T$ the target nucleus mass. As $M_T$ is much bigger than the projectile mass $M_P$ the target recoil potential becomes proportional to $M_P/M_T$ and therefore it can be taken into account perturbatively. This procedure has been adopted here and in fact we assume, with respect to the wavefunction constructions, that the target nucleus remains at rest in the laboratory reference frame.

In order to develop a distorted-wave model let us define the initial wavefunction by means of

$$\mathbb{X}_i^{(+)}(\boldsymbol{R}, \boldsymbol{r}_T) = \chi_{k_i}^{(+)}(\boldsymbol{R})\phi_i(\boldsymbol{r}_T) \tag{3}$$

where $\chi_{k_i}^{(+)}$ is the outgoing nuclear scattering state with initial relative momenta $\boldsymbol{k}_i$ and $\phi_i$ is the initial electronic orbital. $\chi_{k_i}^{(+)}$ is an exact eigenstate of the nuclear Hamiltonian $H_N$; it includes exactly the strong internuclear interaction so that the large-angle deviation is adequately described.

In the same way, we write the exact final wavefunction in the form

$$\Psi_f^{(-)}(\boldsymbol{R}, \boldsymbol{r}_T) = \chi_{k_f}^{(-)}(\boldsymbol{R})\psi_f(\boldsymbol{R}, \boldsymbol{r}_T). \tag{4}$$

Here $\chi_{k_f}^{(-)}$ is the ingoing nuclear scattering state with final relative momenta $\boldsymbol{k}_f$. In writing equation (4) we have been motivated by the following consideration. In the standard small-angle scattering the strong dependence on $\boldsymbol{R}$ of the total wavefunction is contained in the phase factor $\exp(i\boldsymbol{k}_f \cdot \boldsymbol{R})$. Therefore, the substitution $\Psi_f^{(-)}(\boldsymbol{R}, \boldsymbol{r}_T) = \exp(i\boldsymbol{k}_f \cdot \boldsymbol{R})\psi_f(\boldsymbol{R}, \boldsymbol{r}_T)$ leads to the 'electronic wavefunction' $\psi_f$ which varies slowly with $\boldsymbol{R}$. This fact legitimizes the standard approximation $|\nabla_R^2 \psi_f| \ll k_f \|\nabla_R \psi_f\|$ which is valid above a few keV amu$^{-1}$ (Wilets and Wallace 1968, Bransden and Coleman 1972, Flannery and McCann 1973) and leads to the well known semiclassical form of the scattering amplitude. Obviously, this is so because in forward scattering the plane wave adequately describes the nuclear motion. For intermediate energy large-angle scattering the nuclear evolution is adequately described by means of nuclear state $\chi_{k_f}^{(-)}$. Therefore, one expects a slow dependence on $\boldsymbol{R}$ of $\psi_f$ in equation (4) compared with that of $\chi_f^{(-)}$. This fact will be discussed in more detail in section 3. Farther on, we shall show that the function $\psi_f$ is closely related to the semiclassical time-dependent electronic wavefunction. For our present purpose suffice it to say that $\psi_f$ is chosen in order that $\Psi_f^{(-)}$ solves the full quantum Schrödinger equation (18). The distorted initial wavefunction $\mathbb{X}_i^{(+)}$ and the exact final wavefunction $\Psi_f^{(-)}$ are subjected to the asymptotic conditions

$$\mathbb{X}_i^{(+)} \underset{\substack{R\to\infty \\ r_T \text{ finite}}}{\simeq} \exp(i\boldsymbol{k}_i \cdot \boldsymbol{R})\phi_i(\boldsymbol{r}_T) + \text{outgoing waves} \tag{5a}$$

$$\Psi_f^{(-)} \underset{\substack{R_f\to\infty \\ r_P \text{ finite}}}{\simeq} \exp(i\boldsymbol{k}_f' \cdot \boldsymbol{R}_f)\phi_f(\boldsymbol{r}_P) + \text{ingoing waves} \tag{5b}$$

where $\boldsymbol{k}_f'$ is the relative final momentum which is related to $\boldsymbol{k}_f$ by $\boldsymbol{k}_i' = \boldsymbol{k}_f + \boldsymbol{v}_f$, $\boldsymbol{v}_f$ being the final relative velocity. Using the approximate relation $\boldsymbol{R}_f \simeq \boldsymbol{R} + M_P^{-1}\boldsymbol{r}_P$ we can rewrite equation (5*b*) as

$$\Psi_f^{(-)} \underset{\substack{R\to\infty \\ r_P \text{ finite}}}{\simeq} \exp(i\boldsymbol{k}_f\cdot\boldsymbol{R})\phi_f(\boldsymbol{r}_p)\exp(i\boldsymbol{v}_f\cdot(\boldsymbol{r}_p+\boldsymbol{R})) + \text{ingoing waves.} \tag{5c}$$

In the above equations and in those that follow we have neglected terms of the order of $M_P^{-1}$. With this choice, the scattering amplitude $f_{fi}^{ex}$ for the charge exchange process is

$$\begin{aligned} f_{fi}^{ex} &= -\Lambda(2\pi)^{-1}\langle\langle\Psi_f^{(-)}, (H-E)\mathbb{X}_i^{(+)}\rangle\rangle = -\Lambda(2\pi)^{-1}(t_{fi}^C + t_{fi}^R) \\ t_{fi}^C &= \langle\langle\chi_{k_f}^{(-)}\psi_f, V_P\chi_{k_i}^{(+)}\phi_i\rangle\rangle \\ t_{fi}^R &= M_T^{-1}\langle\langle\chi_{k_f}^{(-)}\psi_f, (\mathbb{P}\chi_{k_i}^{(+)})\cdot(\boldsymbol{p}\phi_i)\rangle\rangle \end{aligned} \tag{6}$$

where $\langle\langle\ \rangle\rangle$ denotes a double $\boldsymbol{R}$ and $\boldsymbol{r}_T$ integration. In writing equation (6), we have taken into account the fact that the initial distorting potential (i.e. the projectile–target nucleus potential) cannot produce electron capture by itself. The total energy $E$ can be written using the energy conservation law as

$$E = \frac{k_i^2}{2\Lambda} + \varepsilon_i = \frac{k_f^2}{2\Lambda} + \varepsilon_f + \tfrac{1}{2}v_f^2 \tag{7}$$

where $\varepsilon_i$ and $\varepsilon_f$ are the electronic energies of the initial target and final projectile orbital, respectively.

## 3. The broken straight line approximation

An important fact that helps us in the scattering amplitude calculation is the large difference between the length scales of the nuclear and the atomic phenomena. Following the Blair–Anholt discussion (Blair and Anholt 1982) we assume the existence of a matching radius $R_m$ between the typical atomic and nuclear distances, $R_a$ and $R_n$, respectively. For the systems and resonance energies of interest in this work typical $R_a$ and $R_n$ lengths are $10^{-1}$ and $10^{-4}$, respectively. These typical values can be obtained by calculating the distance of closest approach in a zero impact parameter Coulomb collision and the K-shell radius of the atomic target. The choice $R_m \simeq 5\times10^{-3}$ splits the $\boldsymbol{R}$ integration in an inner region $R < R_m$, inside of which the electronic potential and the atomic wavefunction vary slowly, and an external domain $R > R_m$ where the nuclear wavefunctions have reached their asymptotic values. With these considerations in mind let us rewrite the Coulomb $t$ matrix in the form

$$\begin{aligned} t_{fi}^C &= \int d\boldsymbol{R}\,\chi_{k_f}^{(-)*}(\boldsymbol{R})\chi_{k_i}^{(+)}(\boldsymbol{R})A(\boldsymbol{R}) \\ A(\boldsymbol{R}) &= \int d\boldsymbol{r}_T\,\psi_f^*(\boldsymbol{R},\boldsymbol{r}_T)V_p(\boldsymbol{r}_p)\phi_i(\boldsymbol{r}_T). \end{aligned} \tag{8}$$

The asymptotic nuclear wavefunctions have the explicit forms

$$\begin{aligned} \chi_{k_i}^{(+)as} &= \exp(i\boldsymbol{k}_i\cdot\boldsymbol{R}) + f^{(+)}(\boldsymbol{k}_i,\hat{\boldsymbol{R}})\exp(ik_iR)/R \\ \chi_{k_f}^{(-)as} &= \exp(i\boldsymbol{k}_f\cdot\boldsymbol{R}) + f^{(-)}(\boldsymbol{k}_f,\hat{\boldsymbol{R}})\exp(-ik_fR)/R \end{aligned} \tag{9}$$

where $f^{(+)}$ and $f^{(-)}$ are nuclear scattering amplitudes and $\hat{\boldsymbol{R}}$ denotes the $\boldsymbol{R}$ direction. At this point we can make use of the slow variation of $\psi_f$ with respect to the nuclear coordinate $\boldsymbol{R}$. As we have put forward in section 2, the chief $\boldsymbol{R}$-dependence of the total wavefunction $\Psi_f^{(-)}$ is contained in the nuclear state $\chi_{k_f}^{(-)}$, whose typical wavelength is $\lambda_C = 2\pi/v\Lambda$. In effect, for large-angle scattering at intermediate and high energies the nuclear motion is well described by the nuclear state $\chi_{k_f}^{(-)}$ which exactly takes into account the nucleus–nucleus potential. The $\boldsymbol{R}$-dependence of $\psi_f$ is originated in the nuclei–electron interactions. These nuclei–electron interactions cannot significantly change the nuclear momentum distribution owing to the smallness of the electron–nucleus mass ratio. So the typical $R$ wavelength of $\psi_f$ will be very large compared with $\lambda_C$. This means that $\psi_f$ does not change appreciably when $R$ varies in the nuclear scale. Of course, the electron–nucleus interaction is crucial for the electronic motion and therefore $\psi_f$ will change noticeably with $R$ varying in the atomic scale. With these considerations in mind, let us rewrite the $t$ matrix (8) in the following way:

$$t_{fi}^{C} = \int \mathrm{d}\boldsymbol{R}\, \chi_{k_f}^{(-)*}(\boldsymbol{R}) \chi_{k_i}^{(+)}(\boldsymbol{R})[A(\boldsymbol{R}) - A(0)] \tag{10a}$$

which can be justified by noting that the orthogonality of the nuclear states with $k_i \neq k_f$ cancels the $A(0)$ contribution. The advantage of writing $t_{fi}^{C}$ in the form (10$a$) is that the relevant contribution to the integral comes from the external domain $R > R_m$. In fact, owing to the preceding discussion the 'electronic wavefunction' $\psi_f(\boldsymbol{R}, \boldsymbol{r}_T)$ can be well approximated by $\psi_f(0, \boldsymbol{r}_T)$ for $R < R_m$. Therefore, the bracket in (10$a$) vanishes in the inner region. This permits us to replace the nuclear states for their respective asymptotic forms in (10$a$) to obtain

$$t_{fi}^{C} \simeq \int \mathrm{d}\boldsymbol{R}\, \chi_{k_f}^{(-)\mathrm{as}*}(\boldsymbol{R}) \chi_{k_i}^{(+)\mathrm{as}}(\boldsymbol{R})[A(\boldsymbol{R}) - A(0)]. \tag{10b}$$

In order to carry out the $\boldsymbol{R}$ integration, we can use the large $kR$ approximation of the plane waves in equations (9):

$$\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}) \simeq \frac{2\pi}{\mathrm{i}kR}[\delta(\hat{\boldsymbol{R}} - \hat{k}) \exp(\mathrm{i}kR) - \delta(\hat{\boldsymbol{R}} + \hat{k}) \exp(-\mathrm{i}kR)]. \tag{11}$$

In our case this large $kR$ expansion is useful because the typical $k$ value for the systems under consideration is $10^4$. Then, for $R > R_m$ is valid the inequality $kR > 50$ which legitimizes the use of equation (11). By inserting (9) in (10) and with the help of (11) we obtain four contributions to the $\boldsymbol{R}$ integration. Two of these integrands include the rapidly oscillating factors $\exp(\pm\mathrm{i}(k_f + k_i)R)$ and can be discarded. The factors $\exp(\pm\mathrm{i}(k_f - k_i)R)$ can be integrated over all the directions of $\boldsymbol{R}$ to give, except for the forward direction,

$$t_{fi}^{C} = t_{fi}^{C(\mathrm{in})} + t_{fi}^{C(\mathrm{out})}$$

$$t_{fi}^{C(\mathrm{in}_{\mathrm{out}})} = \frac{-2\pi}{\mathrm{i}k_{i,f}} f^{(+)}(k_{i,f}\hat{k}_i, \hat{k}_f) \int_0^\infty \mathrm{d}R \exp(\pm\mathrm{i}\Delta kR)[A(\mp\hat{k}_{i,f}R) - A(0)] \tag{12}$$

where we have used the time reversal equality $f^{(-)*}(k_f, -\hat{k}_i) = f^{(+)}(k_f\hat{k}_i, \hat{k}_f)$. It must be noted that the broken straight line nuclear trajectory emerges at this point in the $A$-argument $(\mp\hat{k}_{i,f}R)$. Therefore, the values of the $A(\boldsymbol{R})$ (and therefore those of the $\psi_f(\boldsymbol{R}, \boldsymbol{r}_T)$) outside the broken line are not relevant for the $t_{fi}^{C}$ evaluation. The change of the relative nuclear momenta $\Delta k$ can be found from the energy conservation law (7):

$$\Delta k \simeq (k_f^2 - k_i^2)/2k_i = -(\Delta\varepsilon/v + \tfrac{1}{2}v) \tag{13}$$

where $\Delta\varepsilon$ is the change in the orbital electronic energy and $v$ denotes the initial or final collision velocity. In equation (12) and in those that follow the first (second) subindex must be related to the upper (lower) sign. At this point the connection with the semiclassical time-dependent formalism is apparent. In fact, we can rewrite the $R$ integrals carrying out the change of variable $R = \mp vt$, where the upper (lower) sign corresponds to the way in (out). By making this, we obtain

$$t_{fi}^{C} = -2\pi\Lambda^{-1}[f(E_f, \theta)a_{fi}^{C(in)} + f(E_i, \theta)a_{fi}^{C(out)}] \tag{14}$$

where the nuclear scattering amplitudes are $f(E_{i,f}, \theta) = f^{(+)}(k_{i,f}\hat{k}_i, \hat{k}_f)$ and where $\theta$ is the angle between $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ and $E_{i,f}$ are the nuclear energies. The electronic Coulomb amplitudes are

$$a_{fi}^{C(\substack{in\\out})} = \pm i \int_0^{\mp\infty} dt \exp(i(\Delta\varepsilon + \tfrac{1}{2}v^2)t)[A(\hat{v}_{i,f}t) - A(0)]. \tag{15}$$

The above mentioned fact, that the values of $\psi_f(\boldsymbol{R}, \boldsymbol{r}_T)$ outside the broken line $\boldsymbol{R} = \boldsymbol{v}_{i,f}t$ are not relevant at all, permits us to define a new wavefunction restricted to the mentioned broken path. Examination of $A(\boldsymbol{R})$ in equation (8) suggests the following definition of this new broken straight line electronic wavefunction:

$$\psi_f^{BSL}(\boldsymbol{r}_T, t) = \exp(-i(\varepsilon_f + \tfrac{1}{2}v^2)t)\psi_f(\hat{v}_{i,f}t, \boldsymbol{r}_T) \tag{16}$$

where the first (second) subindex corresponds to negative (positive) times. By means of this, the electronic Coulomb amplitudes can be rewritten in the familiar semiclassical form

$$\begin{aligned} a_{fi}^{C(\substack{in\\out})} &= a_{fi}^{C_{as}(\substack{in\\out})} + a_{fi}^{C_{st}(\substack{in\\out})} \\ a_{fi}^{C_{as}(\substack{in\\out})} &= \pm i \int_0^{\infty} dt \langle \psi_f^{BSL}(\boldsymbol{r}_T, t),\ V_p^{(\substack{in\\out})}(\boldsymbol{r}_T, t) \exp(-i\varepsilon_i t)\phi_i(\boldsymbol{r}_T)\rangle \\ a_{fi}^{C_{st}(\substack{in\\out})} &= \mp(\Delta\varepsilon + \tfrac{1}{2}v^2)^{-1}\langle \psi_f^{BSL}(\boldsymbol{r}_T, 0),\ V_p(\boldsymbol{r}_T, 0)\phi_i(\boldsymbol{r}_T)\rangle \end{aligned} \tag{17}$$

where $V_p^{(\substack{in\\out})} = -Z_p/|\boldsymbol{r}_T - \boldsymbol{v}_{i,f}t|$. To obtain the inner correction $a_{fi}^{C_{st}}$ to the Coulomb amplitude (the so-called Coulomb sticking term) we have assumed the existence of a long-range convergence factor in the $R$ coordinate; in fact this has been understood in writing equations (10). The angular bracket notation in (17) denotes the integration over the electronic coordinates.

So far, nothing has been said about the wavefunction $\psi^{BSL}$ except that it is related to $\psi_f$ through equation (16). In order to identify the above amplitudes with the ones that follow from the semiclassical picture, we must prove that the function $\psi_f^{BSL}$ satisfies the time-dependent Schrödinger equation for the prescribed nuclear potential. To this end, we start with the full quantum Schrödinger equation

$$(H - E)\Psi_f^{(-)}(\boldsymbol{R}, \boldsymbol{r}_T) = 0 \tag{18}$$

which leads, by using equation (4), to the following equation for the 'electronic wavefunction $\psi_f$':

$$\begin{aligned} &[H_T + V_P - \boldsymbol{\eta}(\boldsymbol{R})\cdot\nabla_{\boldsymbol{R}} - (2\Lambda)^{-1}\nabla_{\boldsymbol{R}}^2 - (\varepsilon_f + \tfrac{1}{2}v^2)]\psi_f(\boldsymbol{R}, \boldsymbol{r}_T) = 0 \\ &\boldsymbol{\eta}(\boldsymbol{R}) = \Lambda^{-1}\nabla_{\boldsymbol{R}}\chi_{\boldsymbol{k}_i}^{(-)}/\chi_{\boldsymbol{k}_i}^{(-)}. \end{aligned} \tag{19a}$$

Although the $\nabla_{\boldsymbol{R}}$ and $\nabla_{\boldsymbol{R}}^2$ terms both contain the small factor $\Lambda^{-1}$, their orders of magnitude are very different. In effect, the typical momentum of the Coulomb wave

is $\Lambda v$. Therefore the order of magnitude of $\boldsymbol{\eta}$ is the same as that of $v$. In contrast, the small factor $\Lambda^{-1}$ in the $\nabla_R^2$ term is not compensated for, owing to the large typical $R$ wavelength of the function $\psi_f$. This is an 'atomic' wavelength, as has been already discussed in the paragraph following equation (9). So, we can neglect the small fourth term in (19$a$) and write:

$$[H_T + V_P - \boldsymbol{\eta}(\boldsymbol{R}) \cdot \nabla_{\boldsymbol{R}} - (\varepsilon_f + \tfrac{1}{2}v^2)]\psi_f(\boldsymbol{R}, \boldsymbol{r}_T) = 0. \tag{19b}$$

If we make the substitution:

$$\psi_f'(\boldsymbol{R}, \boldsymbol{r}_T) = \exp(i(\varepsilon_f/v + \tfrac{1}{2}v)R)\psi_f(\boldsymbol{R}, \boldsymbol{r}_T) \tag{20}$$

we find, inserting in (19), the following equation for the new wavefunction

$$[H_T + V_P - \boldsymbol{\eta} \cdot \nabla_{\boldsymbol{R}} - (\varepsilon_f/v + \tfrac{1}{2}v)(v + i\boldsymbol{\eta} \cdot \boldsymbol{R})]\psi_f'(\boldsymbol{R}, \boldsymbol{r}_T) = 0. \tag{21}$$

This equation must be integrated only along the broken straight line because the other $\boldsymbol{R}$ values are not relevant for the $t_{fi}^C$ calculation (see the remark following equation (12)). The vector $\boldsymbol{\eta}$ can be calculated by direct derivation of the asymptotic function $\chi_{\boldsymbol{k}_f}^{(-)as}$. For $\boldsymbol{R}$ along the prescribed path, this vector becomes

$$\boldsymbol{\eta}(\boldsymbol{R}) = iv\hat{\boldsymbol{R}} \qquad (\boldsymbol{R} = \mp \hat{v}_{i,f} R) \tag{22}$$

which cancels the contribution of the third term of (21) and permits us to rewrite the gradient term as $iv\partial/\partial R$, where $\partial/\partial R$ is the directional derivative along the broken path. In writing equation (22) for the way out we have used the inequality $|f^{(-)}(\boldsymbol{k}_f, \hat{\boldsymbol{k}}_f)| \ll R_m$. It can be justified by the time reversal invariance $|f^{(-)}(\boldsymbol{k}_f, \hat{\boldsymbol{k}}_f)| = |f^{(+)}(\boldsymbol{k}_f, -\hat{\boldsymbol{k}}_f)|$ that permits us to regard $f^{(-)}$ as a back-scattering nuclear amplitude whose order of magnitude is the same as the typical nuclear distance $R_n$. To write equation (22) for the in way we have used equation (11) in order to discard the plane wave contribution. In both cases, terms of order $\Lambda^{-1}$ have been neglected. Inserting (22) in (21) and using definition (16) and variable $t$, we obtain the time-dependent Schrödinger equation for the electron in the nuclear field:

$$[H_T + V_P^{(\text{in}}_{\text{out})}(\boldsymbol{r}_T, t) - i\partial/\partial t]\psi_f^{BSL}(r_T, t) = 0. \tag{23}$$

This semiclassical equation must be integrated subject to the final condition

$$\psi_f^{BSL}(\boldsymbol{r}_T, t) \underset{t \to \infty}{\simeq} \phi_f(\boldsymbol{r}_P) \exp[i(\boldsymbol{v}_f \cdot \boldsymbol{r}_T - (\varepsilon_f + \tfrac{1}{2}v^2)t)] \tag{24}$$

which follows from (5$c$), (9) and (16).

The preceding results permit us to conclude that the Coulomb $t$ matrix $t_{fi}^C$ can be written, for large angles, as a two-term amplitudes formula: the first term corresponds to the electron capture on the way in with a semiclassical broken straight line amplitude $a_{fi}^{C(in)}$ and a nuclear scattering amplitude $f$, which must be evaluated at the final nuclear energy $E_f = E_i - \Delta E$ because the nuclei make contact with an energy loss $\Delta E = \Delta\varepsilon + \frac{1}{2}v^2$; the second interference term reflects the fact that electron capture can take place on the way out and therefore the semiclassical amplitude $a_{fi}^{C(out)}$ is multiplied by the nuclear scattering amplitude at the initial energy $E_i$. In both cases the electronic evolution has been separated from the nuclear evolution and must be calculated by solving the time-dependent Schrödinger equation for a prescribed broken straight line trajectory. There is a contribution from the inner region (see equation (17)), the Coulomb sticking term, which takes into account the possibility of electron capture during the compound nuclei formation. As can be seen from equation (17) this possibility does not modify the total capture amplitude $a_{fi}^C = a_{fi}^{C(in)} + a_{fi}^{C(out)}$ but it plays an important role in the interference phenomena.

In order to conclude this general semiclassical formalism we must rewrite the target recoil $t$ matrix in the form of a two-amplitude term expression as in the case of the Coulomb contribution. To this end we use the second equality of equation (2), the Hermiticity of the nuclear Hamiltonian $H_N$ and the additional approximation

$$H_N\chi_{k_f}^{(-)}\psi_f \simeq [H_N\chi_{k_f}^{(-)}]\psi_f - \Lambda^{-1}\nabla_R\chi_{k_f}^{(-)}\cdot\nabla_R\psi_f \tag{25}$$

which has been obtained by neglecting the term $(-2\Lambda)^{-1}\chi_{k_f}^{(-)}\nabla_R^2\psi_f$ that does not include the strong $\boldsymbol{R}$ derivation of the nuclear wavefunction. Making this, we obtain from (6)

$$\begin{aligned} t_{fi}^{R} &= t_{fi}^{R1} + t_{fi}^{R2} \\ t_{fi}^{R1} &= \Lambda\Delta E M_T^{-1}\langle\!\langle \chi_{k_f}^{(-)}\psi_f, \chi_{k_i}^{(+)}\boldsymbol{R}\cdot\nabla_{r_T}\phi_i\rangle\!\rangle \\ t_{fi}^{R2} &= -M_T^{-1}\langle\!\langle \nabla_R\chi_{k_f}^{(-)}, \nabla_R\psi_f\cdot\chi_{k_i}^{(+)}\boldsymbol{R}\cdot\nabla_{r_T}\phi_i\rangle\!\rangle. \end{aligned} \tag{26}$$

The calculation of the first term of (26) can be carried out in the same way as in the Coulomb case. Here, the $\boldsymbol{R}$ factor cancels the recoil sticking term. We obtain once more the equation (14) with

$$a_{fi}^{R1(\substack{\text{in}\\\text{out}})} = \pm i\int_0^{\mp\infty} dt\left\langle \psi_f^{BSL}(r_T, t), \frac{\Lambda\Delta E}{M_T}\boldsymbol{R}\cdot\nabla_{r_T}\phi_i(r_T)\exp(-i\varepsilon_i t)\right\rangle. \tag{27}$$

In order to evaluate the second target recoil term we replace the nuclear wavefunctions by their asymptotic forms. By neglecting the two gradient terms which do not contain the large momenta $k_f$ we again obtain a Coulomb-type expression with

$$a_{fi}^{R2(\substack{\text{in}\\\text{out}})} = \mp\frac{(\Delta E+\varepsilon_i)}{\Delta E}a_{fi}^{R1(\substack{\text{in}\\\text{out}})} + i\int_0^{\mp\infty} dt\left\langle i\frac{\partial}{\partial t}\psi_f^{BSL}, \frac{\Lambda}{M_T}\boldsymbol{R}\cdot\nabla_{r_T}\phi_i\exp(-i\varepsilon_i t)\right\rangle. \tag{28}$$

Finally, using the relationship between the $t$ matrix and the scattering amplitude, we can write

$$\begin{aligned} f_{fi}^{ex} &= a_{fi}^{(in)}f(E_i-\Delta E,\theta) + a_{fi}^{(out)}f(E_i,\theta) \\ a_{fi}^{(\substack{\text{in}\\\text{out}})} &= a_{fi}^{C_{as}(\substack{\text{in}\\\text{out}})} + a_{fi}^{C_{st}(\substack{\text{in}\\\text{out}})} + a_{fi}^{R1(\substack{\text{in}\\\text{out}})} + a_{fi}^{R2(\substack{\text{in}\\\text{out}})} \end{aligned} \tag{29}$$

where $a_{fi}^{C_{as}}$ and $a_{fi}^{C_{st}}$ are given by equation (17) and $a_{fi}^{R1}$ and $a_{fi}^{R2}$ are given by equations (27) and (28), respectively.

It must be remarked at this point, that the present formalism is not restricted to the charge exchange process. In fact the only reference to the final state was the asymptotic condition (24) for the exact final wavefunction. Thus we can conclude that there is no formal difference in the theoretical treatment of ionization and electron capture processes and both can be described by the very simple equation (29). We must say that a two-amplitude formula like (29) has been already applied to charge exchange by Horsdal *et al* (1986). In that work its use was justified in the framework of the impulse approximation which essentially describes electron capture as ionization to a definite momentum state of the target continuum. We have shown in the above discussion that the connection with the ionization process is not necessary to generalize the Blair–Anholt formula.

In large-angle measurements of electron capture the quantity of interest is not the differential cross section but the angular electron capture probability. This probability

can be evaluated by means of the ratio

$$P^{ex}(E,\theta)=\frac{d\sigma/d\Omega}{|f(E,\theta)|^2}=\left|a_{fi}^{(in)}\frac{f(E-\Delta E,\theta)}{f(E,\theta)}+a_{fi}^{(out)}\right|^2 \tag{30}$$

where $d\sigma/d\Omega$ is the differential cross section for charge exchange. In writing (30) it is assumed that the elastic scattering is the dominant process so that $|f|^2$ can be regarded as the differential cross section.

## 4. Applications

In this section we apply the preceding semiclassical formalism to the evaluation of electron capture probabilities in the presence of nuclear resonances in order to make a comparison with experimental data. The processes that have been subjected to experimental measurements are

| | | | | | |
|---|---|---|---|---|---|
| (1) | $^{12}C(p,p)^{12}C$ | at $E_R=0.462$ MeV | $\Gamma=35$ KeV | $l=0$ | $J=\frac{1}{2}$ |
| (2) | $^{14}N(p,p)^{14}N$ | at $E_R=1.058$ MeV | $\Gamma=6$ KeV | $l=0$ | $J=\frac{3}{2}$ |
| (3) | $^{20}Ne(p,p)^{20}Ne$ | at $E_R=1.955$ MeV | $\Gamma=4$ KeV | $l=2$ | $J=\frac{5}{2}$ |
| (4) | $^{22}Ne(p,p)^{22}Ne$ | at $E_R=1.510$ MeV | $\Gamma=2.45$ KeV | $l=0$ | $J=\frac{1}{2}$ |

where the resonance energies $E_R$ as well as the widths $\Gamma$ are given in the laboratory reference frame. Also we include the proton angular momenta $l$ and the total angular moment $J$ of each resonance. The first two reactions have been investigated by Scheurer *et al* (1985), the third reaction has been measured by Horsdal *et al* (1986) and the last one by Baker *et al* (1987, 1988).

To evaluate semiclassical electron capture amplitudes we have selected the broken straight line version of the peaking impulse approximation (PIA) (Kocbach and Briggs 1984). This choice is prescribed by practical reasons: firstly, the PIA code is available from previous works (Maidagan and Salin 1987, Maidagan 1988) and it reproduces the general trend of experimental data at intermediate energies for two of the systems of interest here; secondly, the target recoil and the sticking terms can be readily incorporated into the calculation scheme developed in the mentioned works. The PIA model can be obtained by assuming

$$\psi_f^{BSL}\simeq\phi_f(0)\phi_{v_f}^{(-)}(r_T)\exp(-i\tfrac{1}{2}v^2t) \tag{31}$$

where $\phi_{v_f}^{(-)}$ is an ingoing Coulomb state with momentum $v_f$ for all the time. The reader is referred to Kocbach and Briggs (1984) for a physical discussion of this choice and to Maidagan (1988) for the details of the numerical calculation. The sticking and the target recoil contributions can be evaluated without difficulty by employing the techniques developed by Maidagan (1988) ($a_{fi}^{R2}$ cancels for this choice).

The orbitals of the ground states of the target are described by a linear combination of Slater orbitals, as calculated by Clementi and Roetti (1974) in their table 1. The effective target distortion charge of the ingoing Coulomb state $\phi_{v_f}^{(-)}$ has been chosen following the criterion of Belkić *et al* (1979): $Z_{ef}^2=-2n_i^2\varepsilon_i$, where $\varepsilon_i$ and $n_i$ are the energy and the principal quantum number of the initial orbital, respectively. In the description of the resonant nuclear scattering we have used a sum of pure Coulomb

plus Breit-Wigner resonance amplitudes. The scattering amplitude $f$ for the two proton $S_{1/2}$ resonances on $^{12}C$ and $^{22}Ne$ are approximated by

$$f = f_c + \frac{1}{K}\frac{\Gamma/2}{E_R - E - i\Gamma/2}$$

$$f_c = -\frac{\eta}{2K\sin^2(\theta/2)}\exp[-2i\eta\ln(\sin(\theta/2))] \tag{32}$$

$$\eta = \frac{Z_T Z_P}{v}$$

where $\theta$ is the centre of mass angle and $K$ the relative momentum of the nuclei. The resonance parameters for $^{12}C$ have been extracted from Milne (1954) and for $^{22}Ne$ from Keyworth *et al* (1968) and Bloch *et al* (1969). For the proton $S_{3/2}$ resonance on $^{14}N$ it is necessary to take into account the two possibilities for the total angular momentum $J$ which, for $l=0$, can take the values $\frac{1}{2}$ and $\frac{3}{2}$. Neglecting non-resonant scattering with $l \neq 0$ we write, following Hagedorn *et al* (1957),

$$|f|^2 = \tfrac{1}{3}|f_{1/2}|^2 + \tfrac{2}{3}|f_{3/2}|^2$$

$$f_{1/2} = f_c + \frac{1}{K}\exp(i\phi_{1/2})\sin\phi_{1/2}. \tag{33}$$

$$f_{3/2} = f_c + \frac{1}{K}\exp(i\phi_{3/2})\sin\phi_{3/2} + \frac{1}{K}\exp(2i\phi_{3/2})\frac{\Gamma/2}{E_R - E - i\Gamma/2}.$$

where the hard sphere phaseshifts, $\phi_{1/2} = -0.5$ and $\phi_{3/2} = -0.08$, have been taken from the mentioned authors. In order to compare with previous SPB calculations we have used the resonance energy of Ajzenberg-Selove (1981) and the width of Olness *et al* (1958). Finally, in the proton $d_{5/2}$ resonance on $^{20}Ne$ we must take into consideration the spin-flip amplitude (Bloch *et al* 1969) and we write

$$|f|^2 = |f_{\uparrow\uparrow}|^2 + |f_{\uparrow\downarrow}|^2$$

$$f_{\uparrow\uparrow} = f_c + \frac{3}{K}\frac{\Gamma/2}{E_R - E - i\Gamma/2}\exp(i\alpha_2)P_2^0(\cos\theta)$$

$$f_{\uparrow\downarrow} = \frac{1}{K}\frac{\Gamma/2}{E_R - E - i\Gamma/2}P_2^1(\cos\theta) \tag{34}$$

$$\exp(i\alpha_2) = \frac{(2+i\eta)(1+i\eta)}{(2-i\eta)(1-i\eta)}$$

where $P_l^m$ is the associated Legendre polynomial. Experimental data report single-electron capture probabilities from all subshells and so we have used equation (30) for each electronic orbital and nuclear specification. Then we have performed an incoherent sum of the various probabilities (in the $^{14}N$ resonance it is necessary to average over the two $J$ values).

For the $^{12}C$ case which has been experimentally studied by means of $CH_4$, the K shell electron capture is the most relevant process at the resonance energy (Horsdal-Pedersen *et al* 1982). Therefore we have not included the L shell contribution in our calculation. For the $^{14}N$ resonance captures from the 1s and the 2s subshells have been considered while for $^{20}Ne$ and $^{22}Ne$ we have included 1s, 2s and 2p subshells. Even where experimental data refer to electron capture to all projectile states, our calculation includes only capture to 1s projectile state.

In figure 2 we show the calculated transfer probability for protons on $^{12}C$ at $\theta_{lab} = 150°$ in the vicinity of the 0.462 MeV elastic resonance. In this case the ratio $\Delta E/\Gamma \simeq 0.015$ does not predict a resonance effect on capture probability and in fact our calculation shows a small structure across the resonance energy. Experimental data (Scheurer *et al* 1985) as well as previous theoretical SPB results confirm this prediction. In the bottom part of this figure we show the experimental 150°/30° counting rate ratios of Scheurer *et al* (1985) and our calculated elastic nuclear cross section ratio. The experimental counting rate ratios are proportional to the cross section ratios and therefore we have scaled the theoretical curve to fit the experimental magnitudes. Figure 3 is similar to figure 2 but for protons on $^{14}N$ across the 1.058 MeV elastic resonance. For this resonance the ratio $\Delta E/\Gamma$ is approximately 0.16. Despite this small value and the incoherent contribution of the 2s subshell (for which the ratio is 0.10), the experimental and the theoretical data show a noticeable resonance effect. In figure 4 we present results for protons on $^{20}Ne$ at $\theta_{lab} = 30°$ that are in good agreement with the experimental probabilities as measured by Horsdal *et al* (1986). Also we show SPB

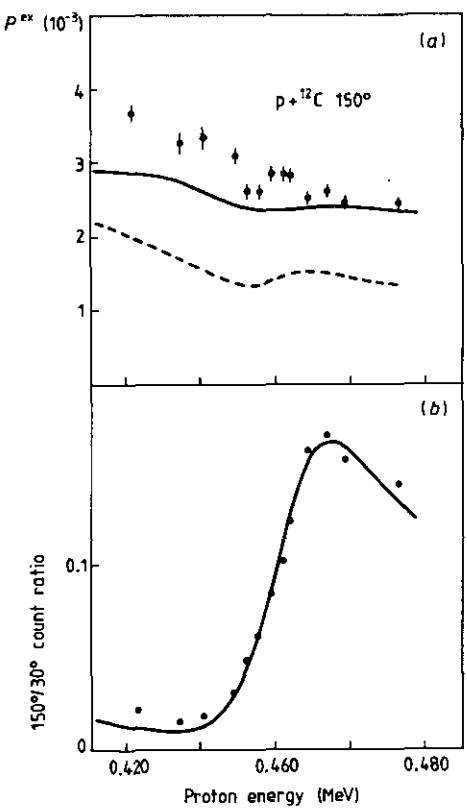


**Figure 2.** (*a*) Electron capture probabilities at $\theta_{lab} = 150°$ for $p+CH_4$ collisions across the 0.462 MeV resonance. Present PIA, ——; SPB, - - - -; experimental data from Scheurer *et al* (1985), ⧫. (*b*) The 150°/30° counting rate ratios for elastic nuclear scattering. Present results (see text), ——; experimental data from Scheurer *et al* (1985) ⧫.

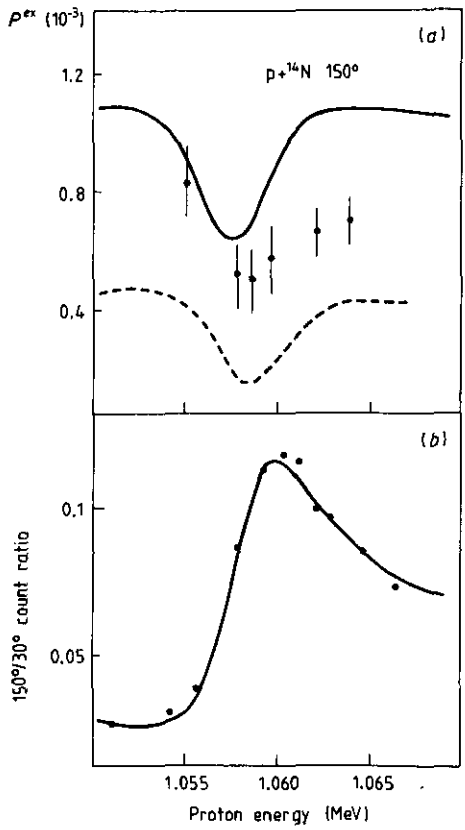


**Figure 3.** Same as for figure 2 but for $p + N_2$ collisions across the 1.058 MeV resonance.

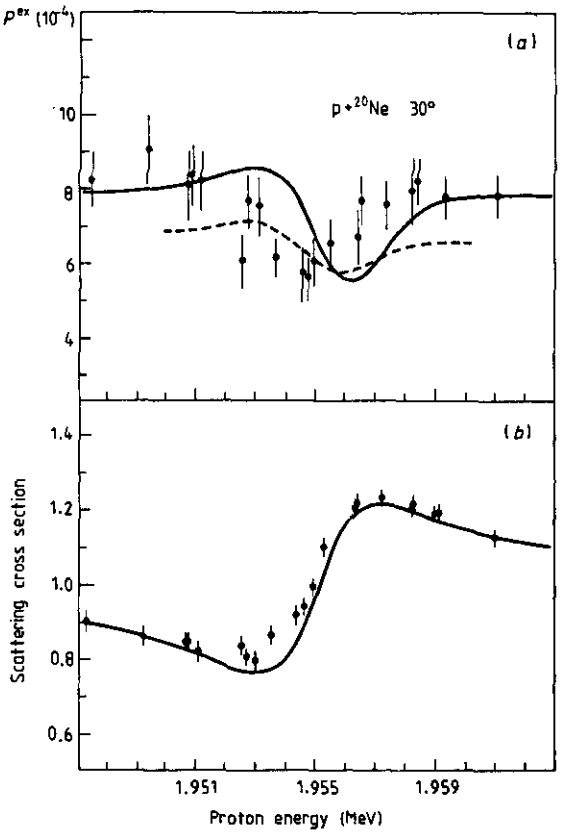


**Figure 4.** (*a*) Electron capture probabilities at $\theta_{lab} = 30°$ for p+$^{20}$Ne collisions across the 1.955 MeV resonance. Present PIA, ——; SPB, - - - -; experimental data from Horsdal *et al* (1986), ●. (*b*) Differential elastic scattering cross sections normalized to the Rutherford cross section. Present results (see text), ——; experimental data from Horsdal *et al* (1986), ●.

probabilities calculated by Jakubassa-Amundsen. The SPB model gives the approximate size of the experimental probabilities but the shape of the measured data is not well reproduced. Both theoretical curves appear slightly shifted in energy with respect to the experimental ones. In the same figure we display the elastic scattering cross section normalized to the Rutherford cross section. Figure 5 exposes the largest discrepancy between experimental data, previous SPB and present PIA calculations. It refers to protons on $^{22}$Ne at $\theta_{lab} = 150°$ and shows the probabilities of charge exchange across the 1.510 MeV elastic resonance. The ratio $\Delta E/\Gamma$ is in this case approximately 0.7 for the K shell and therefore a large interference effect is expected. Experimental data show a broad structure which is not reproduced by theoretical curves. It must be remarked that our calculation does not include the energy spread of the proton beam (2 keV wide). This could explain, in part, the larger structure of the PIA curve compared with the SPB one, which has been corrected to take the spread into account (Baker *et al* 1988). In the bottom part of the same figure we display the 150°/30° elastic nuclear cross section ratio.

Despite the differences in the size of the PIA and SPB probabilities it is apparent by examination of figures 2–5 that there is a qualitative agreement between the

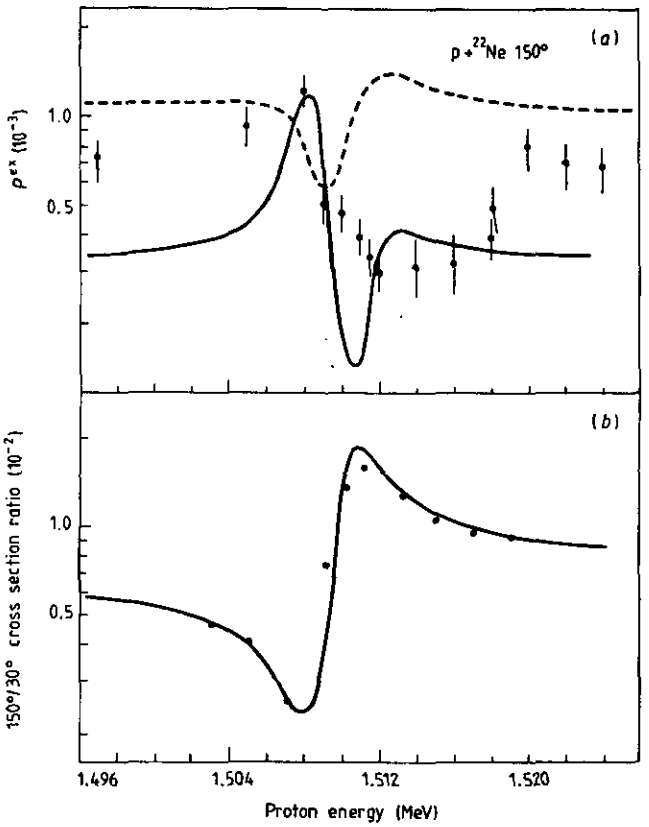


**Figure 5.** (*a*) Electron capture probabilities at $\theta_{lab} = 150°$ for $p + {}^{22}Ne$ collisions across the 1.510 MeV resonance. Present PIA, ——; SPB, - - - -; experimental data from Baker *et al* (1988), ♦. (*b*) The 150°/30° elastic scattering cross sections ratio for 75% of $^{22}Ne$. Present results (see text), ——; experimental data from Baker *et al* (1988), ♦.

calculations. The size of the probabilities is governed by the magnitude of the semiclassical amplitudes so that the above size differences must be attributed to the particular semiclassical description of the electron motion in the approximations. It is clear, in our view, that the simple two-amplitude formula (30) is able to describe the gross features of the experimental capture probability in the presence of a nuclear resonance. We think that the first theoretical task necessary in order to remove the discrepancies between theory and experiment is to improve the descriptions of the electron motion. We know from Baker *et al* (1988) that this procedure cannot lead to agreement with the experimental data for the $^{22}Ne(p, p)^{22}Ne$ resonance. In fact, these authors have carried out unsuccessfully a model calculation based on expression (30). In this case it is necessary to investigate the adequacy of the nuclear scattering amplitude phase given by equation (32).

## 5. Conclusion

We have showed that the simple two-interference Blair–Anholt formula for ionization in the presence of a nuclear resonance can be generalized to electron capture. This

generalization has been obtained from a fully quantum mechanical treatment by performing approximations which are the large-angle counterparts of those used to obtain the forward semiclassical scattering amplitude. This leads to a two-amplitude semiclassical formula for the electron capture probabilities which involves electronic amplitudes that must be calculated for a prescribed broken straight line nuclear trajectory. Application of this simple formula to different systems shows that it is able to describe the gross features of the electron capture across a nuclear resonance. We find a general agreement with previous SPB calculations. The large discrepancy between theory and experimental data for protons on $^{22}$Ne at 1.510 MeV has not been removed.

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