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# Radiative Electron Capture Accompanying Resonant Nuclear Scattering

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A quantum mechanical theory for the radiative capture (REC) of a target electron by a heavy, swift projectile is formulated, allowing for resonant nuclear scattering through the use of distorted waves. Calculations are performed for the systems $O^{16}$, $Ne^{20} \rightarrow He$ within the exact strong potential Born theory and the impulse approximation. Similar structures as in the case of Coulomb capture are found in the transition probability.

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## 1. Introduction

The study of interference effects between atomic excitation and nuclear scattering during the collision of heavy ions has attracted much interest lately. Such investigations are promising because they yield detailed information on the atomic transition amplitudes, allowing in particular for a separation of the contributions to electronic excitation before and after the nuclear interaction and thus for a determination of the relative phases [1]. On the other hand, they have also proven the feasibility of extracting data on nuclear scattering amplitudes and reaction mechanisms [2, 3].

One of the first experimental and theoretical activities has concerned $K$-shell excitation by resonantly scattered protons [1, 3, 4] and recently, resonance structures have also been found in Coulomb capture of target electrons [5, 6]. It is also tentative to interprete structures in the positron spectra from superheavy collision systems in terms of resonant nuclear scattering [7].

Apart from studies concerning the emission of electrons or positrons, also radiation processes have been considered as good candidates to show resonance phenomena. Experimental investigations of nucleus-nucleus bremsstrahlung have revealed structures in the photon spectrum at an impact energy slightly above a nuclear resonance [2, 8]. This process has the advantage that for the observation of interference effects, only a single collision energy is needed, in contrast to inner-shell excitation or charge transfer, where the projectile energy has to be varied across the resonance. These interference effects are most prominent when the energy transfer during the collision coincides with the width of the nuclear resonance.

In this work, the radiative capture of a target electron is investigated when the projectile energy is close to the excitation energy of an isolated resonance. Due to the presence of a peak in the REC spectrum, the identification and separation of REC from background radiation should be easier than in the case of bremsstrahlung. On the other hand such an experiment, which would provide a crucial test for the higher-order theory within which electron capture is formulated, is likely to be less difficult than for Coulomb capture, as the change of the projectile charge need not be detected.

The theoretical description of REC follows closely the methods developped for Coulomb capture [6] (Sect. 2). Both the impulse approximation [9] and the strong potential Born approximation [10] are used for the calculations, and the influence of off-shell effects on the resonance structures and the photon spectra as a function of scattering angle are investigated. The interference structures are studied at fixed photon frequency when the impact velocity is varied across the resonance, as well as in the photon spectrum at fixed collision energy. Numerical results are presented for the collision systems $O^{16} \rightarrow He$ and $Ne^{20} \rightarrow He$ (Sect. 3). A short conclusion is given in Sect. 4. Atomic units ($\hbar = m = e = 1$) are used unless otherwise indicated.

## 2. Quantum Mechanical Description of REC

We restrict ourselves to the capture of a single target electron in the case where the projectile (nuclear charge $Z_P$, mass $M_P$) is much heavier than the target $(Z_T, M_T)$. In the case of fast collisions this process may be viewed as radiative recombination of a quasifree electron in the field of the projectile. Quantum mechanically, the electron is first ejected into an off-shell state $\psi_{\mathbf{q},E_0}$ of the projectile with momentum $\mathbf{q}$ and energy $E_0$ which differs from its on-shell value $q^2/2$ by an amount of the order of the initial binding energy. Subsequently, the electron jumps down into its final projectile state $\psi_f^P$ via photon emission. The exact consideration of the internuclear potential thereby allows for a nuclear scattering between excitation and recombination. This is reflected in the transition amplitude, which in the strong potential Born (SPB) approximation [6, 10] can be written as a folded product of an overlap term and the radiation matrix element

$$W_{fi}=\int d\mathbf{K}\, d\mathbf{q} \langle \psi_f^P(\mathbf{r}_P)\, \chi_{\mathbf{K}_f}^{(-)} |\, H_R | \chi_{\mathbf{K}}^{(+)} \psi_{\mathbf{q},E_0}(\mathbf{r}_P)\rangle \cdot \langle \mathbf{q}(\mathbf{r}_P)\, \chi_{\mathbf{K}}^{(+)} |\, \psi_i^T(\mathbf{r}_T)\, \chi_{\mathbf{K}_i}^{(+)}\, e^{-i\beta\mathbf{K}_i\mathbf{r}_T}\rangle \tag{2.1}$$

where $H_R$ is the radiation field, $\psi_i^T$ describes a bound electronic target state, $|\mathbf{q}\rangle$ is an electronic plane wave with momentum $\mathbf{q}$, and $\mathbf{r}_P$ and $\mathbf{r}_T$ are the electronic coordinates in the projectile and target frame of reference, respectively.
The nuclear scattering states are denoted by $\chi_{\mathbf{K}}^{(\pm)}$ where $\mathbf{K}_i$, $\mathbf{K}$ and $\mathbf{K}_f$ are the initial, intermediate and final internuclear momenta, respectively. Further, we have used the abbreviations

$$H_R=\frac{i}{c}\mathbf{A}_\lambda \nabla_{\mathbf{r}_P}, \quad \mathbf{A}_\lambda=\sqrt{\frac{c^2}{4\pi^2\omega}}\,\mathbf{u}_\lambda$$
$$\beta=\frac{m}{m+M_T}, \quad E_0=E-\frac{K^2}{2\mu_f}, \quad \mu_f=\frac{M_T(M_P+m)}{M_P+M_T+m} \tag{2.2}$$

where $\mathbf{u}_\lambda$ is the polarisation direction of the photon with frequency $\omega$, and $E$ is the total energy of the collision system.
In (2.1), all terms which are small of the order of $Z_T/Z_P$ have been neglected in consistency with the SPB approximation scheme as a first-order theory in the weak target-electron potential.
For the further evaluation use is made of the fact that the length scales of the atomic and nuclear reactions are very different, so that one may split the nuclear wavefunctions $\chi_{\mathbf{K}}(\mathbf{R})$ into an interior part $\chi_{\mathbf{K}}^{in}$ plus the asymptotic scattering solution $\chi_{\mathbf{K}}^{as}$ and assume all atomic transition matrix elements to be constant in the region $R \lesssim R_N$ where $\chi_{\mathbf{K}}^{in}$ deviates appreciably from zero [4, 6]. Actually, when evaluating the overlap term in (2.1), where the atomic part reduces to $\exp(i\mathbf{q}\mathbf{R})\,\varphi_i^T(\mathbf{q}+\beta\mathbf{K}_i)$ with $\varphi_i^T$ the Fourier transform of the initial state $\psi_i^T$, one should rather add the momentum shift $\mathbf{q}$ to the momentum $\mathbf{K}_i$ of $\chi_{\mathbf{K}_i}$ for $R<R_N$ instead of setting $\exp(i\mathbf{q}\mathbf{R})\approx 0$ in that region, as this phase is not weakly dependent on $R$. This approximation is reasonable because the contribution from small internuclear distances $(R<R_N)$ to the transition amplitude is small anyhow, but also because the exact semiclassical expression will emerge as the limiting case. One obtains

$$\begin{aligned}
W &\equiv \langle \mathbf{q}(\mathbf{r}_P)\, \chi_{\mathbf{K}}^{(+)} |\, \psi_i^T(\mathbf{r}_T)\, \chi_{\mathbf{K}_i}^{(+)}\, e^{-i\beta\mathbf{K}_i\mathbf{r}_T}\rangle \\
&= \varphi_i^T(\mathbf{q}+\beta\mathbf{K}_i) \int d\mathbf{R}\, e^{i\mathbf{q}\mathbf{R}}\, \chi_{\mathbf{K}}^{*(+)}\chi_{\mathbf{K}_i}^{(+)} \\
&\approx \varphi_i^T(\mathbf{q}+\beta\mathbf{K}_i) \Big\{ \delta(\mathbf{q}-\mathbf{K}+\mathbf{K}_i) \\
&\quad -\frac{i}{4\pi^2 K} f^{(+)}(\mathbf{K}_i+\mathbf{q}, \vartheta_{\mathbf{K}_i+\mathbf{q},\mathbf{K}}) \cdot \left[\pi\delta(K_i+\mathbf{q}\hat{\mathbf{K}}_i-K)+\frac{i}{K_i+\mathbf{q}\hat{\mathbf{K}}_i-K}\right] \\
&\quad +\frac{i}{4\pi^2|\mathbf{K}-\mathbf{q}|} f^{(+)}(\mathbf{K}_i, \vartheta_{\mathbf{K}_i,\mathbf{K}-\mathbf{q}}) \cdot \left[\pi\delta(K_i+\mathbf{q}\hat{\mathbf{K}}-K)+\frac{i}{K_i+\mathbf{q}\hat{\mathbf{K}}-K}\right]\Big\}
\end{aligned} \tag{2.3 a}$$

where $f(\mathbf{K},\vartheta)$ is the nuclear scattering amplitude, $\vartheta$ is the c.m. scattering angle, and $\hat{\mathbf{K}}$ denotes the direction of $\mathbf{K}$. All terms of higher than first order in the scattering amplitude have been neglected, but also strongly oscillating terms containing the sum of two internuclear momenta, and $q \ll K, K_i$ has been used to discard quadratic terms in $q$. For the radiation matrix element one gets

$$\begin{aligned}
M &\equiv \langle \psi_f^P(\mathbf{r}_P)\, \chi_{\mathbf{K}_f}^{(-)} |\, H_R | \chi_{\mathbf{K}}^{(+)} \psi_{\mathbf{q},E_0}(\mathbf{r}_P)\rangle \\
&= \frac{i}{c}\mathbf{A}_\lambda \langle \psi_f^P(\mathbf{r}_P)|\, \nabla_{\mathbf{r}_P} | \psi_{\mathbf{q},E_0}(\mathbf{r}_P)\rangle \\
&\quad \cdot \left[\delta(\mathbf{K}-\mathbf{K}_f)+\frac{i}{2\pi\mu_f}\,\delta(E_K-E_{K_f})\, f^{(+)}(\mathbf{K}, \vartheta_{\mathbf{K},\mathbf{K}_f})\right]
\end{aligned} \tag{2.3 b}$$

where $E_K=K^2/2\mu_f$. If the initial and final projectile velocities are introduced via $\mathbf{K}_i=\mu_i\mathbf{v}_i$ and $\mathbf{K}_f=\mu_f\mathbf{v}_f$ with $\mu_i=M_P(M_T+m)/(M_p+M_T+m)$, and the conservation of total energy is used

$$E=\frac{K_i^2}{2\mu_i}+E_i^T=\frac{K_f^2}{2\mu_f}+E_f^P+\omega \tag{2.4}$$

where $E_i^T$ and $E_f^P$ are the energies of the bound electronic states $\psi_i^T$ and $\psi_f^P$, respectively, one may express differences of nuclear momenta by means of electronic quantities. Also, terms of the order of

$m/M_T$ (and $M_T/M_P$) can be neglected after the evaluation of nuclear momentum differences, such that for example, $\mu_i - \mu_f \approx 1$. It is then easy to show that the terms of $W$ and $M$ which are independent of the scattering amplitude $f$ and therefore represent forward scattering lead, when inserted into the transition amplitude (2.1), to the semiclassical expression for the differential cross section for the REC process as given by formula (3.2) of Ref. 10.

In order to study resonant nuclear scattering, large-angle deflection has to be considered where only the terms linear in $f$ are important. This contribution to $W_{fi}$, called $W_{fi}^{(1)}$, is obtained from (2.3) to give

$$W_{fi}^{(1)} = -\frac{\mathbf{A}_\lambda}{4\pi c \mu_i} \int d\mathbf{q}\, \varphi_i^T(\mathbf{q}+\mathbf{v}_i) \langle \psi_f^P | V_{\mathbf{r}_P} | \psi_{\mathbf{q}, E_0} \rangle \cdot \Big\{ f^{(+)}(\varepsilon_f, \vartheta)\, \delta\Big(\Delta E + \frac{v^2}{2} + \mathbf{q}\mathbf{v}_i\Big) - f^{(+)}(\varepsilon_i + \mathbf{q}\mathbf{v}_i, \vartheta) \frac{i}{\pi} \frac{1}{\Delta E + v^2/2 + \mathbf{q}\mathbf{v}_i} + f^{(+)}(\varepsilon_i, \vartheta) \Big[ \delta\Big(\Delta E + \frac{v^2}{2} + \mathbf{q}\mathbf{v}_f\Big) + \frac{i}{\pi} \frac{1}{\Delta E + v^2/2 + \mathbf{q}\mathbf{v}_f} \Big] \Big\}$$

$$\varepsilon_i = K_i^2/2\mu_i, \qquad \varepsilon_f = \varepsilon_i - \Delta E - v^2/2 \qquad (2.5)$$

where the scattering angle $\vartheta$ is the angle between $\mathbf{v}_i$ and $\mathbf{v}_f$, and $v \equiv v_i = v_f$ has been used as we are restricting ourselves to elastic scattering. Further, $\Delta E = E_f^P - E_i^T + \omega$ and the off-shell energy $E_0 = E_f^P + \omega$. The first term in the curly brackets which is proportional to $f^{(+)}(\varepsilon_f, \vartheta)$, describes the photon emission before the nuclear scattering, while the last term ($\sim f^{(+)}(\varepsilon_i, \vartheta)$) describes the REC process after the nuclear interaction. The remaining term denotes excitation before, but radiation after the nuclear scattering. In the case of resonant scattering where $f$ contains a contribution of the structure (3.1), the interference effects between these terms will be largest when the energy transfer $\varepsilon_i - \varepsilon_f$ equals the width $\Gamma$ of the resonance.

The probability for the emission of a photon into the solid angle $d\Omega_\gamma$ can be obtained by means of

$$\frac{d^2 P}{d\omega\, d\Omega_\gamma} = N_i \sum_\lambda \frac{\omega^2}{c^3} \frac{(4\pi^2 \mu_i)^2}{|f^{(+)}(\varepsilon_i, \vartheta)|^2} |W_{fi}^{(1)}|^2 \qquad (2.6)$$

where the sum extends over the two polarisation directions, and $N_i$ is the number of electrons in the initial state $\psi_i^T$. An explicit evaluation of (2.6) in the case of $K-K$ capture is given in the appendix.

From (2.5) the semiclassical limit is readily derived. If no nuclear resonance is present, such that the scattering amplitude depends only weakly on energy ($f(\varepsilon_i, \vartheta) \approx f(\varepsilon_f, \vartheta)$), it can be considered as a common factor of $W_{fi}^{(1)}$. The semiclassical result is then found from multiplying $W_{fi}^{(1)}$ by $-4\pi^2 \mu_i / f^{(+)}(\varepsilon_i, \vartheta)$. It coincides with the formula for the transition amplitude which is obtained by means of integrating the electronic transition matrix element over the classical internuclear trajectory if this trajectory is approximated by a zero impact parameter, broken-line path. This semiclassical calculation can be done along the same lines as for Coulomb capture [11].

## 3. Numerical Results

We have concentrated on the capture of electrons from He by bare $O^{16}$ and $Ne^{20}$ projectiles, and considered only capture into the projectile $K$-shell as this is the dominant process at large impact velocities. For He, hydrogenic wavefunctions with an effective charge 1.7 and binding energy 0.91795 a.u. have been used. The photon ejection angle has been taken $\theta_\gamma = 90°$.

In the case of an isolated resonance with given angular momentum $l$, the amplitude for elastic scattering consists of the Coulomb amplitude plus a resonant term $f_{\text{res}}$ which is assumed to have a Breit-Wigner shape

$$f_{\text{res}}(K, \vartheta) = -\frac{1}{2K}(2l+1)\, e^{2i\sigma_l} P_l(\cos\vartheta) \frac{\Gamma_P}{\varepsilon - E_R + i\Gamma/2} \qquad (3.1)$$

where $\sigma_l$ is the Coulomb phase shift, $P_l$ a Legendre polynomial, $\Gamma_P$ the partial width which in the cases considered equals the total width $\Gamma$. $E_R$ is the resonance energy in the center of mass frame.

Figure 1 shows the capture probability for impinging oxygen near the $l=1$ resonance at $E_R = 4.002$ MeV with width $\Gamma = 2.5$ keV [12]. The width is somewhat larger than the energy transfer $\Delta E + v^2/2 = 1.4$ keV at the REC peak ($\omega_{\text{peak}} = v^2/2 - E_f^P + E_i^T = 1.5$ keV). A resonance structure is seen at fixed $\omega$ when the projectile energy is varied across the nuclear resonance. Apart from a small shift in the position of the extrema, there is only a weak dependence on the photon energy in the vicinity of the REC peak. Thus the finite experimental energy resolution will not destroy the resonance effect. However, similar as for Coulomb capture, the structure is strongly dependent on scattering angle (Fig. 2) because of the interference between the Coulomb part and the resonant part of the scattering amplitude. As the influence of the Coulomb amplitude decreases with increasing $\vartheta$, the resonance effect is most pronounced at large scattering angles except

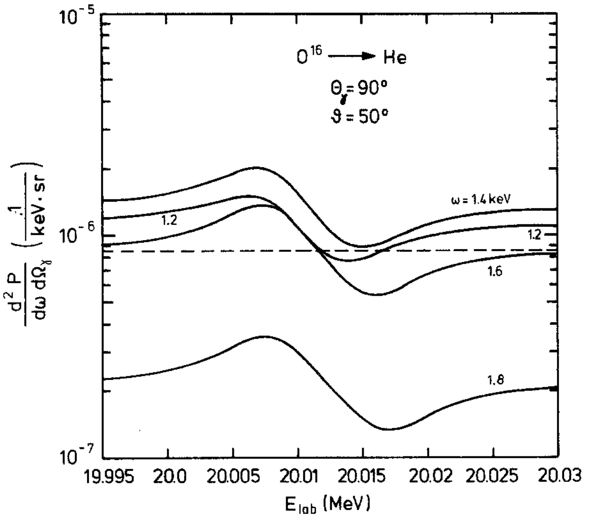


**Fig. 1.** Probability for photon emission during electron capture from He into the $K$-shell of $O^{16}$ as a function of the projectile energy. The scattering angle $\vartheta$ is 50° and the photon emission angle $\theta_\gamma$ is 90°. Shown are SPB calculations at different photon frequencies $\omega$ (full curves) and in the case of $\omega = 1.6$ keV also the result if no nuclear resonance is present (broken curve)

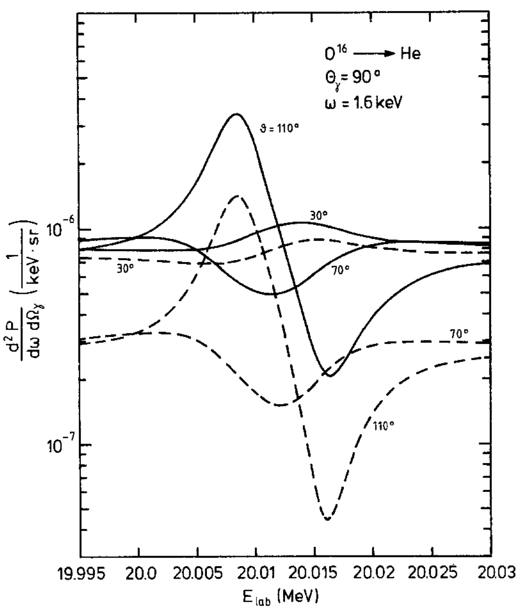


**Fig. 2.** Probability for photon emission during electron capture from He into the $K$-shell of $O^{16}$ as a function of the projectile energy. The photon energy is 1.6 keV and the emission angle 90°. Shown are calculations within the SPB (full curves) and within the IA (broken curves). The scattering angle is taken as parameter

near the zeros of $P_l(\cos\vartheta)$. We have also studied other resonances in this collision system with much larger widths (up to ten times the energy transfer), and also there, a structure was clearly seen, although smaller than in the case discussed above.

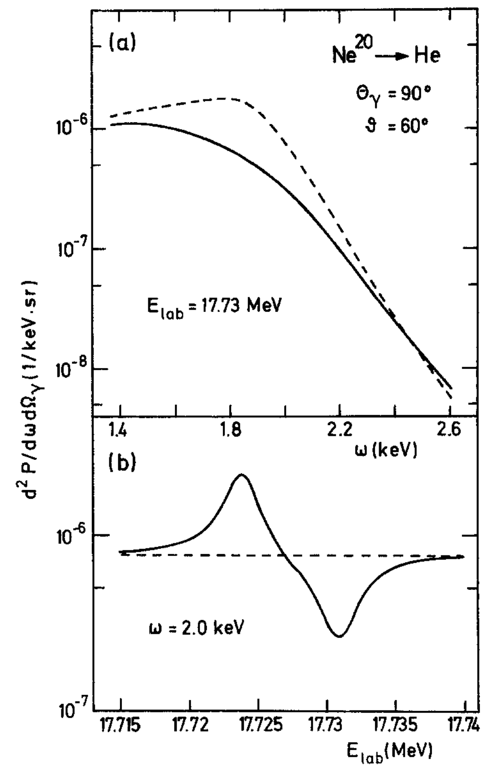


**Fig. 3 a and b.** Probability for photon emission during electron capture from He into the $K$-shell of $Ne^{20}$ at a scattering angle of 60° and photon emission angle of 90°. Shown are SPB calculations with (full curves) and without (broken curves) the presence of a nuclear resonance. The probability is plotted as a function of photon frequency at fixed projectile energy (**a**) and as a function of projectile energy at a given frequency (**b**)

In order to look for structures in the photon spectrum, we have studied the collision system $Ne^{20}$ + He near the $l = 3$ resonance at $E_R = 2.954$ MeV with a rather small width of $\sim 1$ keV [13]. In analogy to bremsstrahlung emission, an interference structure is expected in the photon spectrum, if the energy $\varepsilon_f$ of the outgoing projectile is equal to the resonance energy [8]. From the expression for the energy transfer, the structure should occur at $\omega = \varepsilon_i - E_R - (E_f^P - E_i^T + v^2/2)$, and it should be most pronounced, if $\varepsilon_i - E_R \simeq \Gamma$. For the chosen collision system, this $\omega$ lies slightly above the REC peak ($\omega_{\text{peak}} = 1.8$ keV), and the structure is expected to extend over a range of $\sim 2\Gamma$ around this value of $\omega$. As is shown in Fig. 3a, the resonance effects reveal themselves only in a shift of the peak energy together with a slight modification of the peak shape, as compared to the case when no resonance is present, in contrast to the clear resonance structure if the projectile energy is varied (Fig. 3b). This different behaviour from the bremsstrahlung spectra lies in the fact that the REC spectrum has a very strong de-

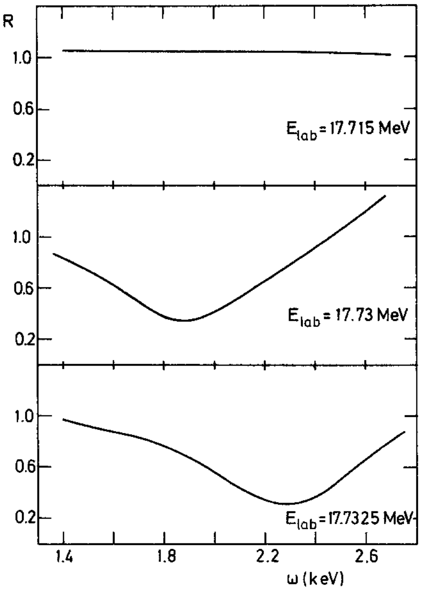


**Fig. 4.** Ratio between SPB calculations with and without the presence of a nuclear resonance for the collision parameters as given in Fig. 3 as a function of photon frequency. The projectile energies correspond to $E_R - 2\Gamma$, $E_R + \Gamma$ and $E_R + 1.5\Gamma$, where in the lab frame, $E_R \triangleq 17.725$ MeV and $\Gamma \triangleq 5$ keV

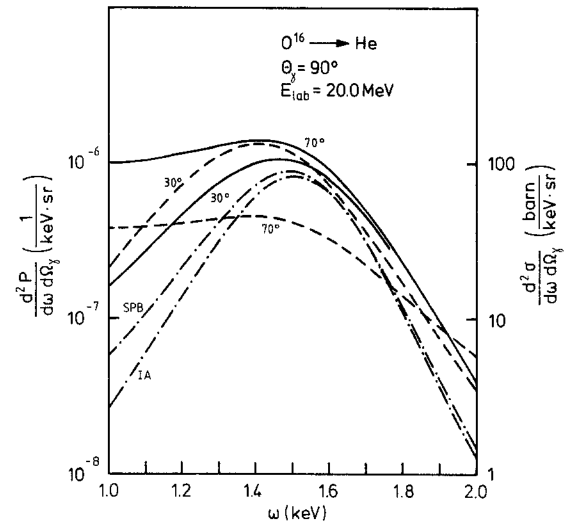


**Fig. 5.** Probability for photon emission during electron capture from He into the $K$-shell of $O^{16}$ as a function of photon energy. The projectile energy is 20 MeV and the photon emission angle 90°. Full curves denote SPB, broken curves IA calculations at two different scattering angles. Also shown is the differential cross section within both theories (chain curves), where the scale is given on the right hand side of the figure

pendence on $\omega$ which is determined by the Compton profile of the bound target electron. Thus, at a frequency $\omega_{\text{peak}} + \Gamma$, the intensity has already decreased by several orders of magnitude. As is shown in Fig. 4, the resonance structure is only evident in the ratio $R$ between the photon emission probability $d^2P/d\omega d\Omega_\gamma$ calculated with and without the presence of a resonant term in the scattering amplitude. The resonance structure in $R$ persists if $\varepsilon_i - E_R$ equals up to $3\Gamma$ or more, but it is correspondingly shifted to higher frequencies. We would like to point out that not only an experimental detection of the modulations in the spectrum will be impossible in these cases, but also that an atomic theory such as SPB becomes invalid for frequencies away from the peak region [10, 14]. For collision energies below $E_R$, no structure exists (cf. Fig. 4).

Even for the optimised condition where the structure is near the REC maximum, experimental detection will be very difficult. The reason is partly the required sharp beam energy (with a spread of at most 1 keV in the above case), but mainly the angular resolution of the particle detector. For $Z_P \gg Z_T$, large differences in the c.m. scattering angle correspond to very small differences in the lab angle. As – in contrast to the case when the projectile energy is varied – the modulations of the REC peak exist only in a rather narrow angular range, they are likely to be washed out in an experimental situation.

We have also investigated the difference between the two current theories for charge transfer, the SPB approximation, and the impulse approximation (IA) which is obtained from (2.5) when the off-shell function $\psi_{q,E_0}$ is replaced by a projectile Coulomb wave. In contrast to Coulomb capture, an exact evaluation poses no problems in the case of REC. Judging from the results for the (angle-integrated) differential cross sections, the two theories agree rather well, especially on the high-energy side of the REC peak [10]. Figure 5 reveals, however, that this is no longer true for the transition probability at large scattering angles. When the frequency is taken at a value where the SPB and IA differential cross sections coincide, $d^2P/d\omega d\Omega_\gamma$ shows a different angular dependence of the two theories (see also Fig. 2). The reason lies in the fact that for large scattering angles, the average momentum transfer $\tilde{q}$ is higher than for near-zero scattering angles (where it is roughly given by $\tilde{q} = (\Delta E + v^2/2)/v$; cf. (2.5)). A larger $\tilde{q}$ is, however, related to smaller spacial distances in the radiation matrix element, and it is at the smallest distances, where on-shell and off-shell wavefunctions differ most. Also in the resonance region there are large deviations between SPB and IA, which vary not only with scattering angle, but also with photon energy. Although the position of the resonance maxima and minima is unaffected (depending primarily on the scattering amplitude itself), the intensity is different, and the structures are larger when the IA is used. This may be due to the fact that the off-shell functions in the SPB theory imply a sum over projectile eigenstates in the intermediate state (and not just a single state as in the IA) which could lead to some washing out of the resonance effect.

## 4. Conclusion

The theory of radiative electron capture has been extended to include distorted nuclear waves which allow for the description of interference effects when the projectile is scattered resonantly off the target. In a similar way as for Coulomb capture, the resulting time-delay between radiation before and after the nuclear interaction causes a resonance structure in the transition probability when the collision energy is varied across the resonance. However, the rapid fall-off of the photon intensity beyond the REC peak makes the visibility of a structure in the photon spectrum itself nearly impossible. Nevertheless, due to the unproblematic separation of the REC photons from the background in the peak region, and due to the fact that only one final electronic state contributes, allowing for a definite energy transfer and thus a sharp structure when the projectile energy is varied, the radiative electron capture from light targets such as H or He, is likely to be a promising tool for the investigation of nuclear reaction phenomena.

As far as theory is concerned, REC has the advantage of being describable with a relatively simple calculation as the transition operator is separable in space and time. Thus it should be feasible to incorporate nuclear scattering states which allow for more general resonances than just isolated ones. On the other hand, the possibility of fast numerical calculations without any additional peaking approximations provides also a stringent test of the atomic theories. The calculations have shown that off-shell effects become rather important at large scattering angles. Since they are related to the influence of the weak target field, one might question whether additional couplings to the target potential could introduce significant changes in the transition probability even in the REC peak region provided the scattering angles are very large. REC is a realistic candidate for going beyond the SPB approximation scheme.

## Appendix

In this appendix, the probability for photon emission is evaluated in the special case of the transfer of a target $K$ electron into the projectile $K$-shell.

It is convenient to decompose $W_{fi}^{(1)}$ from (2.5) into three parts, $W_{fi}^{(1)}=W_{fi}^{A}+W_{fi}^{B}+W_{fi}^{C}$, where $W_{fi}^{A}$ and $W_{fi}^{B}$ denote the terms containing $\delta(\Delta E+v^2/2+\mathbf{q}\mathbf{v}_i)$ and $\delta(\Delta E+v^2/2+\mathbf{q}\mathbf{v}_f)$, respectively, while $W_{fi}^{C}$ collects the principal value terms.

For the evaluation of $W_{fi}^{A}$ and $W_{fi}^{C}$, the quantisation axis is chosen along $\mathbf{v}_i$ which implies that the two photon polarisation directions are given by $\mathbf{u}_1=(0,1,0)$ and $\mathbf{u}_2=(-\cos\theta_\gamma,0,\sin\theta_\gamma)$ if the photon is ejected into the direction $(\sin\theta_\gamma,0,\cos\theta_\gamma)$. As the dipole matrix element is given by [9]

$$\langle\psi_f^P|\nabla_{\mathbf{r}_P}|\psi_{\mathbf{q},E}\rangle=\mathbf{q}\,\frac{2^{3/2}Z_P^{5/2}}{\pi N_0}\,M_f(q) \tag{A.1}$$

$$\begin{aligned}M_{1s}(q)=&\frac{i}{(Z_P^2+q^2)^2}+\frac{Z_P^2}{\eta}\,\frac{1}{FD_1(B^2-C)^{1/2}}\\&\cdot\left[-{}_2F_1\left(1,1-i\eta,2-i\eta,\frac{1}{\rho_+}\right)\frac{1}{(1-i\eta)\,\rho_+}\right.\\&\cdot\left(\frac{BB'}{B^2-C}+i\eta\frac{\rho_+'}{\rho_+}\right)\\&+\left({}_2F_1(1,i\eta,1+i\eta,\rho_-)\frac{1}{i\eta}+\frac{\pi i}{\sinh\pi\eta}(-\rho_-)^{-i\eta}\right)\\&\cdot\left.\left(\frac{BB'}{B^2-C}+i\eta\frac{\rho_-'}{\rho_-}\right)-\frac{\rho_+'}{\rho_+(\rho_+-1)}-\frac{\rho_-'}{\rho_-(1-\rho_-)}\right]\end{aligned}$$

(with the definitions from Ref. 9) where the direction $\hat{\mathbf{q}}$ factors out there remains no contribution from $\mathbf{u}_1$ after the integration over the azimuthal angle $\varphi_q$ for an initial target state which is independent of $\varphi_q$. Inserting the momentum distribution of a $1s$ state, one finds

$$\begin{aligned}W_{fi}^{A}&=-\frac{2(Z_PZ_T)^{5/2}}{\pi^3\sqrt{\omega}\,\mu_i\,v N_0}\,\tilde{W}^A\,\delta_{\lambda,2}\\\tilde{W}^A&=f^{(+)}(\varepsilon_f,\vartheta)\sin\theta_\gamma\\&\quad\cdot\int_{q_{\min}}^{\infty}q^2\,dq\cos\vartheta_q\,M_{1s}(q)\frac{1}{(Z_T^2+q^2+v^2+2\mathbf{q}\mathbf{v}_i)^2}\\q_{\min}&=|\Delta E+v^2/2|/v,\\\mathbf{q}\mathbf{v}_i&=qv\cos\vartheta_q=-(\Delta E+v^2/2).\end{aligned} \tag{A.2}$$

For the term $W_{fi}^{B}$, the quantisation axis is taken along $\mathbf{v}_f$. Thus, $\mathbf{v}_i=v(-\sin\vartheta,0,\cos\vartheta)$ and after the corresponding rotation, $\mathbf{u}_2=(-\cos(\theta_\gamma-\vartheta),0,\sin(\theta_\gamma-\vartheta))$. For the integration over $\varphi_q$, the formulas are needed

$$\begin{aligned}&\int_0^{2\pi}d\varphi_q\frac{1}{(\alpha_0+\beta_0\cos\varphi_q)^2}=\frac{2\pi\alpha_0}{(\alpha_0^2-\beta_0^2)^{3/2}};\\&\int_0^{2\pi}d\varphi_q\frac{\cos\varphi_q}{(\alpha_0+\beta_0\cos\varphi_q)^2}=-\frac{2\pi\beta_0}{(\alpha_0^2-\beta_0^2)^{3/2}}\\&\alpha_0=Z_T^2+q^2+v^2+2qv\cos\vartheta\cos\vartheta_q,\\&\beta=-2qv\sin\vartheta\sin\vartheta_q\end{aligned} \tag{A.3}$$

and again, only $\mathbf{u}_2$ contributes. Thus

$$W_{fi}^B = -\frac{2(Z_P Z_T)^{5/2}}{\pi^3 \sqrt{\omega}\,\mu_i v N_0}\,\tilde{W}^B \delta_{\lambda,2}$$

$$\tilde{W}^B = f^{(+)}(\varepsilon_i, \vartheta) \int\limits_{q_{\min}}^{\infty} q^2\,dq M_{1s}(q)(\alpha_0^2-\beta_0^2)^{-3/2} \cdot [\alpha_0 \cos\vartheta_q \sin(\theta_\gamma-\vartheta) + \beta_0 \sin\vartheta_q \cos(\theta_\gamma-\vartheta)]. \tag{A.4}$$

Into the remaining term, $W_{fi}^C$, enters the scattering amplitude at a $\mathbf{q}$-dependent energy. Neglecting this $\mathbf{q}$-dependence in the Coulomb amplitude and writing the resonant part (3.1) in the form $f_{\rm res}(\varepsilon_i+\mathbf{q}\mathbf{v}_i, \vartheta) = \lambda_0/(\varepsilon_i + qv\cos\vartheta_q - E_R + i\Gamma/2)$, both $\vartheta_q$ and $\varphi_q$ integrations can be performed in the contribution to $W_{fi}^c$ which is independent of $\mathbf{v}_f$, by means of fractal decomposition of the three-product denominator. In the other contribution to $W_{fi}^C$, containing $(\Delta E + v^2/2 + \mathbf{q}\mathbf{v}_f)^{-1}$, only the $\varphi_q$ integral can be performed with the help of the relation

$$P\int\limits_0^{2\pi} d\varphi_q \frac{\cos\varphi_q}{C_0 + B_0\cos\varphi_q} = \frac{2\pi}{B_0}\left[1 - \frac{|C_0|}{\sqrt{C_0^2 - B_0^2}}\,\Theta(|C_0|-|B_0|)\right]$$

$$x = \cos\vartheta_q, \quad C_0 = \Delta E + v^2/2 + qvx\cos\vartheta,$$
$$B_0 = qv\sqrt{1-x^2}\sin\vartheta \tag{A.5}$$

where $\Theta$ is the unit step function. After insertion into (2.6) one finally obtains for the transition probability

$$\frac{d^2P}{d\omega\, d\Omega_\gamma} = \frac{128(Z_P Z_T)^5 \omega}{\pi^2 v^2 c^3 |N_0|^2 |f^{(+)}(\varepsilon_i, \vartheta)|^2} \cdot \Bigg| \tilde{W}^A + \tilde{W}^B - \frac{i}{\pi}\sin\theta_\gamma \int\limits_0^\infty q^2\,dq M_{1s}(q) \cdot \Bigg\{ \frac{f^{(+)}(\varepsilon_f, \vartheta)}{(Z_T^2+q^2-2\Delta E)^2}\left[\frac{2}{Z_+ Z_-}(Z_T^2+q^2+v^2) \cdot (Z_T^2+q^2-2\Delta E) + \frac{\Delta E + v^2/2}{qv} \ln\left|\frac{Z_+(\Delta E + v^2/2 - qv)}{Z_-(\Delta E + v^2/2 + qv)}\right|\right]$$

$$- \frac{\lambda_0}{\varepsilon_f - E_R + i\Gamma/2}\left[\frac{2}{Z_+ Z_-}\frac{Z_T^2+q^2+v^2}{Z_T^2+q^2+v^2-2E_1} + \frac{E_1}{qv(Z_T^2+q^2+v^2-2E_1)^2}\ln\frac{Z_+(E_1-qv)}{Z_-(E_1+qv)}\right]\Bigg\}$$

$$+ \frac{i}{\pi} f^{(+)}(\varepsilon_i, \vartheta)\int\limits_0^\infty q^2\,dq M_{1s}(q) \cdot \int\limits_{-1}^{1} dx \frac{1}{(Z_T^2+q^2+v^2+2qvx)^2}\left[-\frac{\cos\theta_\gamma}{\sin\vartheta} + \left(\frac{C_0\cos\theta_\gamma}{\sin\vartheta} + qvx\sin\theta_\gamma\right)\frac{\operatorname{sign} C_0}{\sqrt{C_0^2-B_0^2}}\,\Theta(|C_0|-|B_0|)\right]\Bigg|^2 \tag{A.6}$$

with the abbreviations

$$E_1 = \varepsilon_i - E_R + i\Gamma/2, \qquad Z_\pm = Z_T^2 + (q \pm v)^2.$$

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