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PEAKING APPROXIMATIONS IN ATOMIC SCATTERING PROBLEMS

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ABSTRACT

A particular peaking approximation used by Kang and Foland (1967) to evaluate a Coulomb Born matrix element is shown to badly misrepresent their total and differential cross sections for the 1s - 2s transition in atomic hydrogen at low impact energies.

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In recent years peaking approximations have been used to evaluate difficult integrals in several different models in atomic scattering theory. Vainshtein et al. (1963) used one in the Vainshtein approximation. All subsequent calculations in the Vainshtein approximation and its modifications (see e.g. Crothers 1967) include a peaking approximation. Akerib and Borowitz (1961) and Coleman and McDowell (1966) used it in an impulse approximation calculation of direct excitation by proton impact and Kang and Foland (1967) used it to evaluate a Coulomb Born matrix element in their recent paper.

In brief a peaking approximation implies the argument that if $f(x)$ is a slowly varying function and $F(x)$ is a function with dominant maximum at $x = x_0$ then

$$\int f(x)\,F(x)\,dx \simeq f(x_0)\int F(x)\,dx \,. \qquad (1)$$

Clearly this is a simple version of the method of stationary phase or of steepest descents (Morse and Feshbach 1953) but omitting any pretense of mathematical

rigor. Use of such an argument will be referred to below as a peaking approximation.

Although this approach has proved useful in calculating radiation induced transition probabilities in atoms, see for instance Schiff (1955), its validity in connection with most atomic scattering problems is doubtful. The above mentioned authors applied it to complicated integrands whose exact behavior is difficult to analyze. It is necessary to consider each case individually and until the total integrand is exactly evaluated it is impossible to know if the peaking approximation is useful in that particular case.

The Vainshtein cases are being investigated by one of us (H.L.K.) but conclusive results have not yet been obtained. Coleman (1968) demonstrates that, for proton impact excitation of atomic hydrogen in the impulse approximation, the peaking approximation gives total cross sections which may be as much as a factor of 10 in error. In this note we show that in Kang and Foland's theory the peaking approximation badly misrepresents the true behavior of the $1s \rightarrow 2s$ excitation matrix element for atomic hydrogen.

Kang and Foland (1967) introduced a new scheme for calculating cross sections for the excitation and ionization of atoms and ions by electrons, which is essentially an extension of the Coulomb-Born approximation. We do not here wish to discuss at length the validity or usefulness of this scheme, but we do wish to touch on one point. In dealing with the excitation of neutral hydrogen by electrons they represent the incident and scattered electrons by Coulomb waves.

These waves do not (asymptotically) properly represent the physical situation. Using these Coulomb Born matrix elements they predict finite excitation probabilities at threshold. The fact is that Coulomb Born matrix elements between hydrogenic bound states automatically yield finite excitation cross sections at threshold. However one must physically justify the use of such matrix elements in the case of neutral atoms. It should be noted that Damburg and Gailitis (1963) showed that atomic hydrogen excitation cross sections arising from electron impacts are finite at threshold because of coupling effects between degenerate quantum states, and not because the scattered electron wave function is Coulombic.

Our chief concern however is with the peaking approximation used by Kang and Foland in evaluating the non-exchange term of their excitation matrix element $T_{i,f}$, where

$$T_{i,f} = \left\langle x_a^{(-)}\left(\underline{k}_1\right)\phi_b(f)\,|V_{ab}|\,x_a^{(+)}\left(\underline{k}_0\right)\phi_b(i)\right\rangle \cdot \qquad (2)$$

Here $\underline{k}_0$ and $\underline{k}_1$ are the wave vectors of the incident and scattered, a, electron; $\phi_b(i)$ and $\phi_b(f)$ are the hydrogenic eigen states of the bound, b, electron, and $V_{ab} = 1/r_{ab}$ is the interaction potential. The "in" and "out" state, attractive Coulomb wave functions of the incident electron are

$$x_a^{(+)}\left(\underline{k}_0\right) = N_0\, e^{i\underline{k}_0\cdot\underline{r}_a} F\left(i/k_0,\ 1,\ ik_0 r_a - i\underline{k}_0\cdot\underline{r}_a\right),$$

$$x_a^{(-)}\left(\underline{k}_1\right) = N_1\, e^{i\underline{k}_1\cdot\underline{r}_a} F\left(-i/k_1,\ 1,\ -ik_1 r_a - i\underline{k}_1\cdot\underline{r}_a\right) \qquad (3)$$

with

$$|N_i|^2 = 2\pi \Big/ \left[k_i \left(1 - e^{-2\pi/k_i}\right)\right] .$$

Kang and Foland show that the direct (non-exchange) excitation amplitude in their theory may be put in the form

$$T_{i,f} = N_1^* N_0 \left(\frac{1}{2\pi^2}\right) \int \frac{e^{i(\underline{q}-\underline{k})\cdot\underline{r}_a}}{k^2} G(\underline{k})\, F\left(\underline{k}_0, \underline{r}_a\right) F^*\left(\underline{k}_1, \underline{r}_a\right) d\underline{r}_a\, d\underline{k} \qquad (4)$$

where $G(\underline{k})$ is the generalized oscillator strength, and $F\left(\underline{k}_i, \underline{r}\right)$ is one of the confluent hypergeometric functions given in (3), and $\underline{q} = \underline{k}_0 - \underline{k}_1$. Since the integral with respect to $\underline{r}_a$ increases without limit as $\underline{k} \to \underline{q}$, they argue that (4) may be replaced by

$$T_{i,f}^{(0)} = N_1^* N_0 \left(\frac{1}{2\pi^2}\right) G(\underline{q}) \int \frac{e^{i(\underline{q}-\underline{k})\cdot\underline{r}_a}}{k^2} F\left(\underline{k}_0, \underline{r}_a\right) F^*\left(\underline{k}_1, \underline{r}_a\right) d\underline{r}_a\, d\underline{k} . \qquad (5)$$

This can be put in the form of a Nordseick integral (Nordseick 1954)

$$T_{i,f}^{(0)} = G(\underline{q})\, N_1^* N_0 \left(I_N\right)_{\lambda \to 0} ,$$

$$I_N = \frac{2\pi}{\alpha} e^{-\pi/k_0} \left(\frac{\alpha}{\gamma}\right)^{i/k_0} \left(\frac{\gamma+\delta}{\gamma}\right)^{-i/k_1} F\left(1 - \frac{i}{k_0}, \frac{i}{k_1}, 1, \frac{\alpha\delta - \beta\gamma}{\alpha(\gamma+\delta)}\right) \qquad (6)$$

with

$$\alpha = \frac{1}{2}\left(q^2 + \lambda^2\right), \qquad \beta = \underline{k}_1 \cdot \underline{q}$$

$$\gamma = \underline{k}_0 \cdot \underline{q} + i\lambda k_1 - \alpha, \qquad \delta = k_0 k_1 + \underline{k}_1 \cdot \underline{k}_0 - \beta,$$

and is their version of the peaking approximation to the matrix element, though they have used a standard transformation to write the hypergeometric function in (6) in an alternative form. Alternative peaking approximations, which differ appreciably from (6) may be derived by noting that the slowly varying factor is $k^{-2} G(\underline{k})$ rather than simply $G(k)$, for example.

Gailitis (1966) has shown that for s - s transitions (4) may be evaluated without approximation, in closed form. We obtain for the 1s → 2s function

$$T_{1s,2s} = \frac{4\sqrt{2}\,Z}{27} N_0 N_1^* \left\{ -\frac{\partial I_N}{\partial \lambda} + \beta_0 \frac{\partial 2 I_N}{\partial \lambda^2} \right\}_{\lambda=\beta_0} \tag{7}$$

with Z being the nuclear charge, and $\beta_0 = 3Z/2a_0$, and a_0 is the Bohr radius.

We have evaluated the non-exchange contribution to the 1s → 2s differential cross section in the Kang-Foland model using both (6) and (7). The results for the differential cross section $I(\theta)$ are shown in Fig. 1, the first Born results being given for comparison; (though it is of doubtful value in this energy range.) The results are shown as a function of scattering angle $\theta = \cos^{-1}\left(\hat{\underline{k}}_0 \cdot \hat{\underline{k}}_1\right)$ at energies W = 1.01 and W = 2.0 threshold units (W = 1.0 ≡ 0.75 Ry). Near threshold the Kang-Foland method differs markedly from the first Born approximation, giving values of $I(\theta)$ an order of magnitude larger in the backward di-

rection. The effect of the peaking approximation is to underestimate by more than a factor of 10 at $\theta = 0$, but to overestimate by 20% in the backward direction. At W = 2 the peaking approximation introduces a spurious maximum in $I(\theta)$ at 40°, and is generally in error by factors of two or three for $\theta < 90°$.

In Table 1 we compare total $1s \rightarrow 2s$ excitation cross sections obtained from (6) and (7) with the 1s - 2s - 2p close coupling results [Damburg and Gailitis (1963), Omidvar (1964), Burke et al. (1967)]. The Kang-Foland model gives results which are approximately a factor of three higher near threshold ($W < 1.15$) than the 3-state close coupling results, while the peaking approximation introduces an additional error of about a factor of two. At higher energies ($W \gg 10$) both (6) and (7) give total cross-sections in close agreement with the first Born approximation.

We conclude that use of a peaking approximation in the evaluation of matrix elements involving Coulomb functions is not in general justified, and may lead to order of magnitude errors. All results reported to date in the Vainshtein approximation should be treated with suspicion until a detailed analysis of the effect of the peaking approximation in that model has been carried out.

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TABLE CAPTION

Table I. $(1s \rightarrow 2s)$ excitation cross sections for atomic hydrogen in units of (πa_0^2). The 3-state close coupling results (c.c.) are from (a) Damburg and Gailitis (1963) and (b) Burke, Ormonde and Witaker (1967). The Coulomb Born results compare the exact solution of Eq. (7) with its approximate solution, Eq. (6), obtained by use of the peaking approximation (P.A.). The close coupling calculations of course take account of exchange but the other calculations do not.

FIGURE CAPTION

Fig. 1 The effect of the peaking approximation on the differential cross section $I(\theta)$ for the $1s \rightarrow 2s$ transition in atomic hydrogen. Energy is given in terms of threshold units (W = 1.0 = 0.75 Ry), (a) W = 1.01, (b) W = 2.0. The curves are 1-first Born approximation; 2-Coulomb-Born, Eq. (7); 3-peaking approximation to the Coulomb-Born, Eq. (6).

Table I

$W = k_0^2/I_{ex}$	c.c.	Coulomb Born	
		Exact	P. A.
1.01	0.174[a]	0.573	1.13
1.50	0.36[b]	.396	..82
2.00	0.25[b]	.301	.62

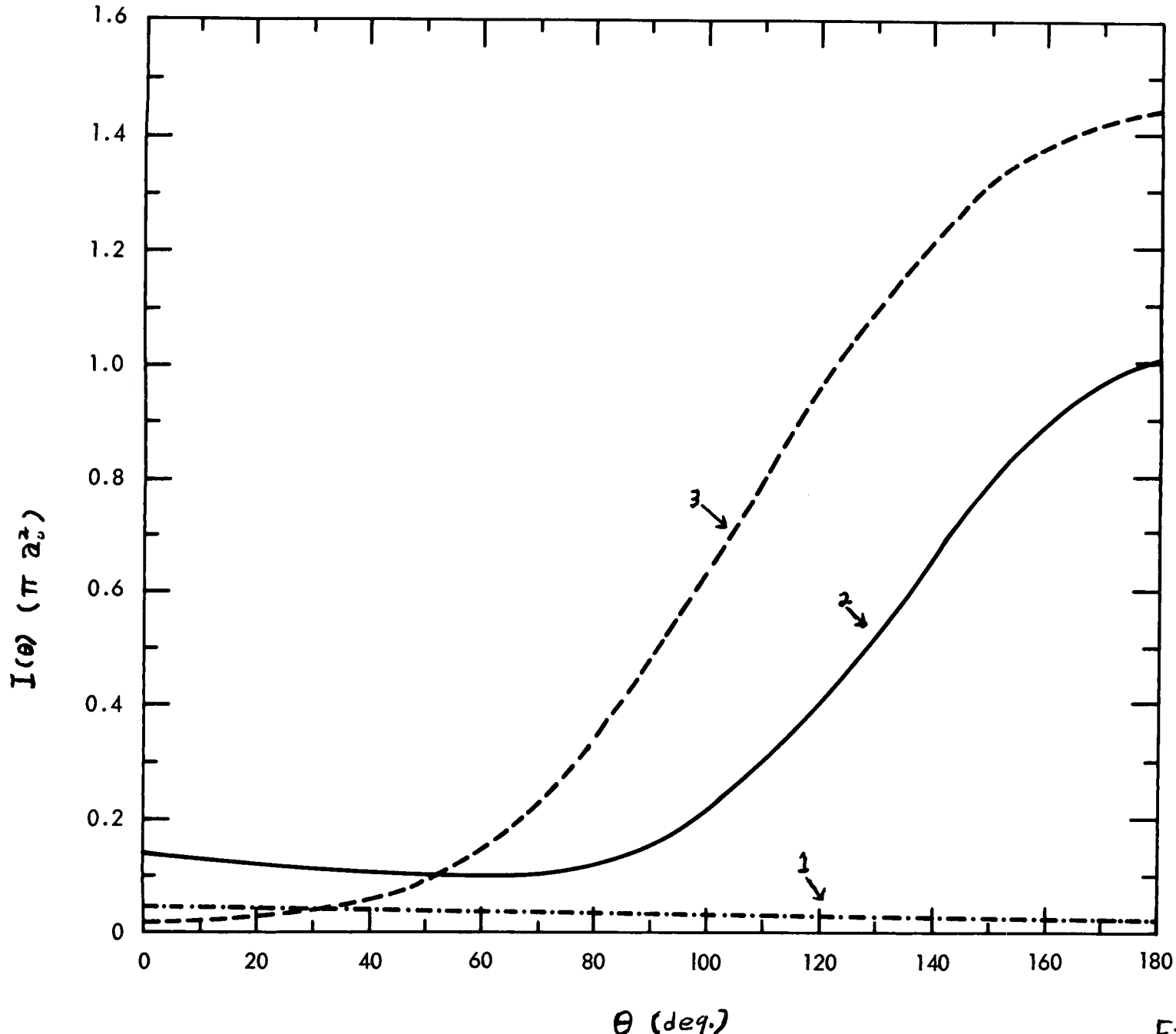
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
I(θ) (π a₀²)
0
20
40
60
80
100
120
140
160
180
θ (deg.)
1
2
3

Fig. 1a

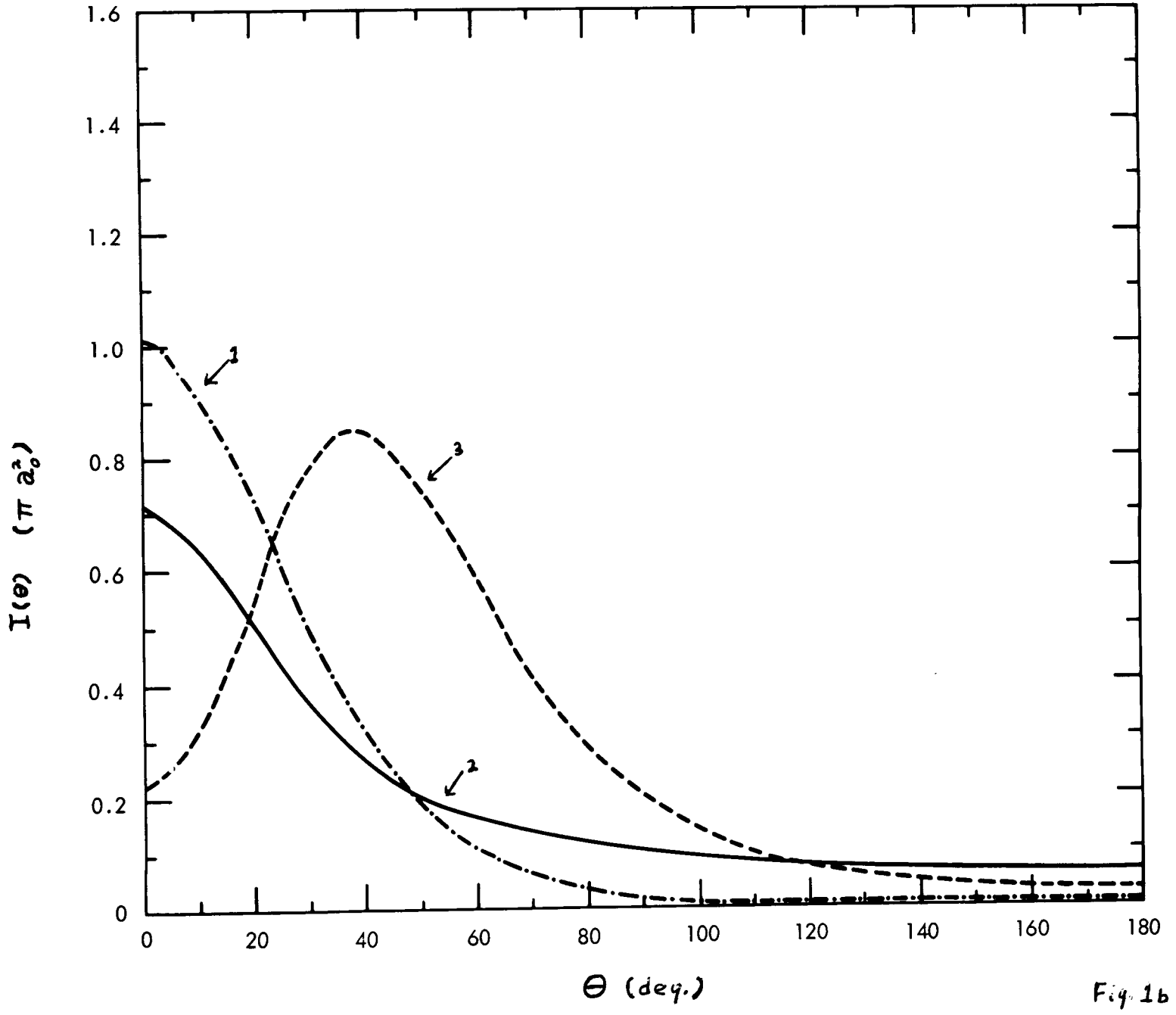
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
I(θ) (π a₀²)
0
20
40
60
80
100
120
140
160
180
Θ (deg.)
1
2
3

Fig. 1b