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#### R. Donangelo, M. W. Guidry, J. P. Boisson, and J. O. Rasmussen

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LBL-4347 Rev.

## THE CLASSICAL-LIMIT S-MATRIX FOR COULOMB EXCITATION R. Donangelo, M. W. Guidry, J. P. Boisson and J. O. Rasmussen

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#### ABSTRACT

An expression for the classical-limit S-matrix for Coulomb excitation is derived and directly evaluated without resorting to stationary phase integration methods. The results obtained are in quantitative agreement with quantum mechanical calculations. This agreement and the simplicity of the method suggest the feasibility of extending it to cases where other methods are not easily applied.

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The electromagnetic interaction occurring in the collision of a nuclear projectile with a deformed target nucleus excites rotational states of the target. Until several years ago only light projectile ions were available, and coupled channel quantum mechanical calculations of the Coulomb excitation process are feasible in this case.

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With the advent of very heavy projectiles exact quantum mechanical calculations have become impractical for the existing computer codes. However, the shortness of de Broglie wavelength for heavy ions brings the problem closer to the realm of classical mechanics. Semiclassical theories use this fact to find approximate solutions to the problem, such as in the Alder-Winther method<sup>1</sup> which is the foundation for the widely used Winther-deBoer code for Coulomb excitation.<sup>2</sup> Recently a quite different approach, the Uniform Semi-Classical Approximation (USCA) developed mainly by Miller,<sup>3,4</sup> was applied to this problem.<sup>5,6</sup>

In this paper we adapt and modify the formalism developed by Marcus,  $^{7-9}$  so that we can study the Coulomb excitation process, and we show its relationship in this case with the USCA as applied in Refs. 5 and 6.

We take as a target a deformed even-even nucleus in its ground state, so that its initial spin is equal to zero and the final spin quantum number I is an even integer.

For simplicity we restrict ourselves to the head-on collision case so that the total angular momentum of the system (target + projectile) is zero. By taking the z-axis along the initial direction of the projectile motion the projection of the target angular momentum on this axis is always equal to zero, and it need not be considered explicitly in our calculations.

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Let  $H_{o}$  be the Hamiltonian of the system for distances large compared to the distance of closest approach;  $H_{o}$  consists then of the kinetic energy of the system plus the long-range Coulomb interaction term. Let  $|\phi_{I}\rangle$  be the eigenstate of  $H_{o}$  in the exit channel corresponding to spin quantum number I of the target for the boundary conditions mentioned before.

At short distances the Hamiltonian is  $H = H_0 + V$ , where V includes the remaining terms of the electromagnetic interaction. We designate by  $|\psi^+\rangle$  the scattered part of the eigenstate of H corresponding to the initial conditions previously given, and evaluated at a time long after the interaction has taken place.

From the usual definition of the S-matrix

$$S_{I \leftarrow O} \equiv \langle \phi_{I} | \psi^{+} \rangle = \int \langle \phi_{I} | q \rangle \langle q | \psi^{+} \rangle dq \qquad (1)$$

where q is a convenient representation and the integration is over all the q space.

Since we do not know the function  $\psi^+(q) = \langle q | \psi^+ \rangle$ , we approximate it with the generalized multidimensional WKB wavefunction

$$\overline{\psi}^{+}(\underline{q}) = A(\underline{q}) \exp \left\{ i \frac{\phi(\underline{q})}{\hbar} \right\} ,$$
 (2)

where, as may be seen in Ref. 7, A conserves probability flux and the phase  $\phi$  satisfies a Hamilton-Jacobi equation.

While in Eq. (1) it was not important which representation was chosen, such is not the case in Eq. (2), since for some choices of

coordinates the WKB wavefunction  $\bar{\psi}^+(q)$  breaks down. Marcus<sup>8,9</sup> gives considerable attention to this problem, and we refer to his papers for additional details.

To test this approach for the Coulomb excitation problem we start by taking the following coordinates to describe our system in the outgoing asymptotic region: X, the angle between the symmetry axis of the target and the line joining the centers of projectile and target and r, the distance between these centers. We denote by L the angular momentum of the target, by  $P_r$  the relative radial momentum and by v the relative velocity. To obtain  $\overline{\psi}^+$  trajectories are run at a given total energy with the initial conditions: r large,  $\chi=\chi_o$  (various arbitrary values), and L = 0. From the values of the dynamical variables in the final asymptotic region we can determine A and  $\phi$ , as shown in Ref. 7. In this  $(\chi, r)$  representation they are given by:

$$= \sqrt{\frac{1}{2} \frac{\sin \chi_{o}}{\sin \chi} \frac{d\chi_{o}}{d\chi} \frac{v_{o}}{v} \cdot \frac{1}{r}}$$
(3)

and

$$p = -\int (r(t)dp_r(t) + \chi(t) dL(t)) + rp_r + \chi L , \qquad (4)$$

where in Eq. (3) quantities with subscript zero are initial values, and quantities without subscript are values at the end of the trajectory. The integral in Eq. (4) is performed along the trajectory. In the asymptotic region  $\phi_{T}$  is given by:

$$\phi_{I} \equiv \langle \underline{q} | \phi_{I} \rangle = \frac{1}{2\pi} \sqrt{\frac{v_{I}}{v_{o}} \left( I + \frac{1}{2} \right)} P_{I}(\cos \chi) \frac{1}{r} e^{i \left[ p_{r} r / \hbar - \eta \ln \left( 2 p_{r} r / \hbar \right) \right]}$$
(5)

where  $v_0$  and  $v_1$  are the asymptotic relative velocities for the values O and I respectively of the target spin quantum number,  $P_1$  is an ordinary Legendre polynomial and n is the Sommerfeld parameter for the exit channel.

Primarily because  $\chi$  does not take a constant value in this asymptotic region, it is not possible to define a good WKB wavefunction in this  $q = (\chi, r)$  representation. Hence, we transform it to a representation analogous to the one in Ref. 9 which is in this case

$$\bar{\chi} = \chi - \omega \tau \quad , \tag{6}$$

here  $\omega$  is the angular velocity of the target at the end of the interaction, and  $\tau$  is the time it would take the projectile to describe an elastic trajectory governed by the Hamiltonian H<sub>o</sub> for an energy equal to that of the projectile on the outgoing asymptotic branch of its actual trajectory. The time  $\tau$  is measured from the point of closest approach on this elastic trajectory to the distance r corresponding to the angle  $\chi$  on the actual trajectory.

In the same way as in Ref. 8 we can show from Eq. (1) that in this case the S-matrix is given by

$$S_{I \leftarrow O} = \int \phi_{I}^{*} \overline{\psi}^{+} 2\pi r^{2} \sin \overline{\chi} \, d\overline{\chi} = \int_{0}^{\pi} \phi_{I}^{*} \overline{\psi}^{+} 2\pi r^{2} \sin \overline{\chi} \, \frac{d\overline{\chi}}{d\chi_{O}} \, d\chi$$

(7)

Or, more explicitly:

$$S_{I \leftarrow 0} = \frac{\sqrt{2I + 1}}{2} \int_{0}^{\pi} P_{I}(\cos \bar{\chi}) \sqrt{\sin \chi_{o} \sin \bar{\chi} \frac{d\bar{\chi}}{d\chi_{o}} \frac{v_{I}}{v_{o}}} e^{i\phi'} d\chi_{o}$$
(8)

where:

$$\phi' = -\frac{1}{\hbar} \int (r(t) dp_r(t) + \chi(t) dL(t)) + \frac{1}{\hbar} \overline{\chi}L + \eta \ln (2p_r r/\hbar)$$

We will examine Eq. (8) in more detail.

First, let us consider the sudden impact limit of a case in which only the quadrupole moment of the target contributes to the excitation. In this limit  $\bar{\chi} = \chi_0$ , and  $\phi' = 2q \sin^2 \chi_0$  where q is given by Eq. (5.11) of Ref. 1: therefore, Eq. (8) reduces to the expression found by Alder and Winther for this same case.<sup>1</sup> This result is very interesting due to the conceptually different approach we have taken.

If we now take the asymptotic expression for the Legendre polynomials

$$P_{I}(\cos\bar{\chi}) \approx 2\cos\left[(I + 1/2) \,\bar{\chi} - \frac{\pi}{4}\right] / \sqrt{(2I + 1) \sin\bar{\chi}}$$

and utilize the fact that initial orientation angles  $\chi_0$  and  $\pi - \chi_0$  result in opposite final angular momenta, we find

$$S_{I+O} \approx \frac{1}{\sqrt{\pi}} \int_{0}^{\pi} \sqrt{\sin\chi_{o} \frac{d\bar{\chi}}{d\chi_{o}} \frac{v_{I}}{v_{o}}} e^{i[\phi' - (I + 1/2)\bar{\chi}]} d\chi_{o}$$
(8')

The evaluation of this integral by the stationary phase approximation results in the USCA as applied in Ref. 6. The weighting factors introduced through geometrical arguments in that paper, and also the use of the I + 1/2 spin quantization condition are thus derived as an approximation of Eq. (8).

We have applied Eq. (8) to several cases. In Fig. 1 we compare our calculations with those obtained by means of the coupled-channel quantum-mechanical code AROSA.<sup>10</sup> In all three cases the agreement is good, especially considering that in these cases the systems considered are not very classical. The method employed here should become more accurate for heavy-ion systems in which the de-Broglie wavelength of the projectile is shorter and the angular momentum transfer becomes larger. No comparison is possible here for those cases, since quantummechanical calculations for heavy systems are not yet feasible. We should remark at this point that the validity of Eq. (8) is limited to cases where the WKB wavefunction  $\bar{\psi}^+$  given in Eq. (3) is a good asymptotic approximation to the actual wavefunction  $\psi^{\dagger}$ . In particular this requires that  $\overline{\chi}$  be a monotonic function of  $\chi_{\alpha}$ ; if not,  $\overline{\psi}^{+}$  will break down at the points where  $\frac{d\bar{\chi}}{d\chi_{2}} = 0$ . These difficulties were not present in any of the calculations presented here, but Kreek et al.<sup>11</sup> reported them for a related problem, and one should be careful that the representation  $\overline{\chi}$  is monotonic in  $\chi_{_{\rm O}}.$ 

Equation (8) is applicable at energies around the Coulomb barrier by including the complex nuclear potential in the equations of motion in the manner of Ref. 13.

The fact that the stationary phase approximation is not used makes Eq. (11) more straightforward to use than the USCA in cases where the stationary phase points are not easy to locate, or where there are more than two of them. Since in our direct integration of Eq. (8) the stationary phase approximation is not used, there is even reason to think that our results could be more precise than those of USCA, especially

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in cases where the exponent in the integrand of Eq. (11) varies slowly. For comparison purposes we give in Table 1 the results obtained by all the methods we have mentioned for one case where this exponent varies slowly. The USCA used is the form using Airy functions as considered in Ref. 6; for this case the Bessel uniform approximation given by Stine and Marcus<sup>12</sup> should be more appropriate. However, the results shown in Ref. 11 indicate that an integral expression such as Eq. (8) is more accurate than the Bessel approximation for the cases shown there.

Finally, we would like to point out that in cases where more than one internal degree of freedom is considered, such as in rotationalvibrational excitation, it may be considerably easier to evaluate directly an expression of the form of Eq. (8) than to perform the multidimensional root search required by all methods based on the stationary phase approximation.

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	(a) $b$					

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Spin	This Work (Eq. 8)	arosa <sup>10</sup>	Winther-deBoer <sup>2</sup>	usca <sup>6</sup>
0	0.1023	0.0890	0.1087	0.1167
2	0.4615	0.4754	0.4375	0.4928
4	0.3571	0.3522	0.3544	0.3336
6	0.0734	0.0775	0.0885	0.0531
8	0.00468	0.00756	0.0103	0.00395

Table 1. Excitation probabilities of rotational levels in  ${}^{168}$ Er for backscattering of 45 MeV  ${}^{10}$ Be.

#### FIGURE CAPTION

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Fig. 1.



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